Advanced Deep Learning

DATA.ML.230

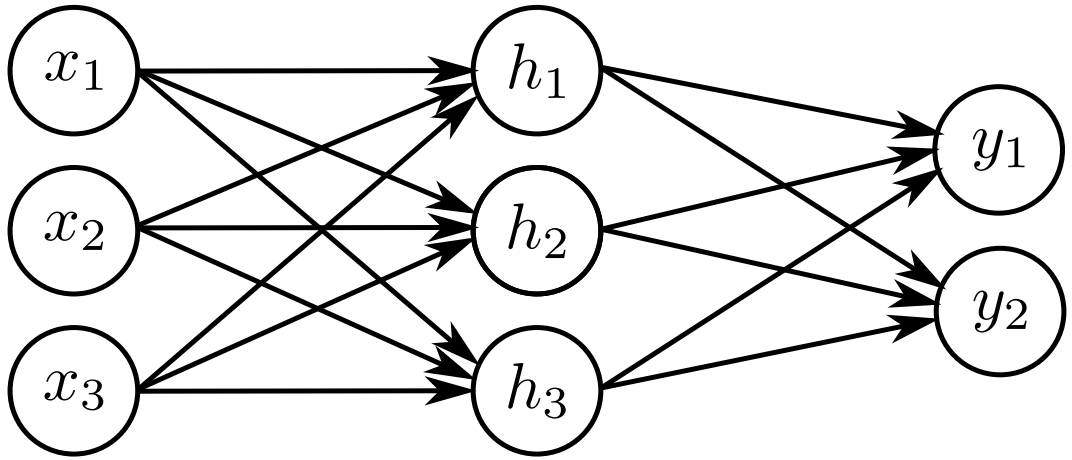
Loss functions

From: Simon J. D. Prince, Chapter 5 – Understanding Deep Learning, MIT Press (19 May 2025)

Shallow Neural Networks

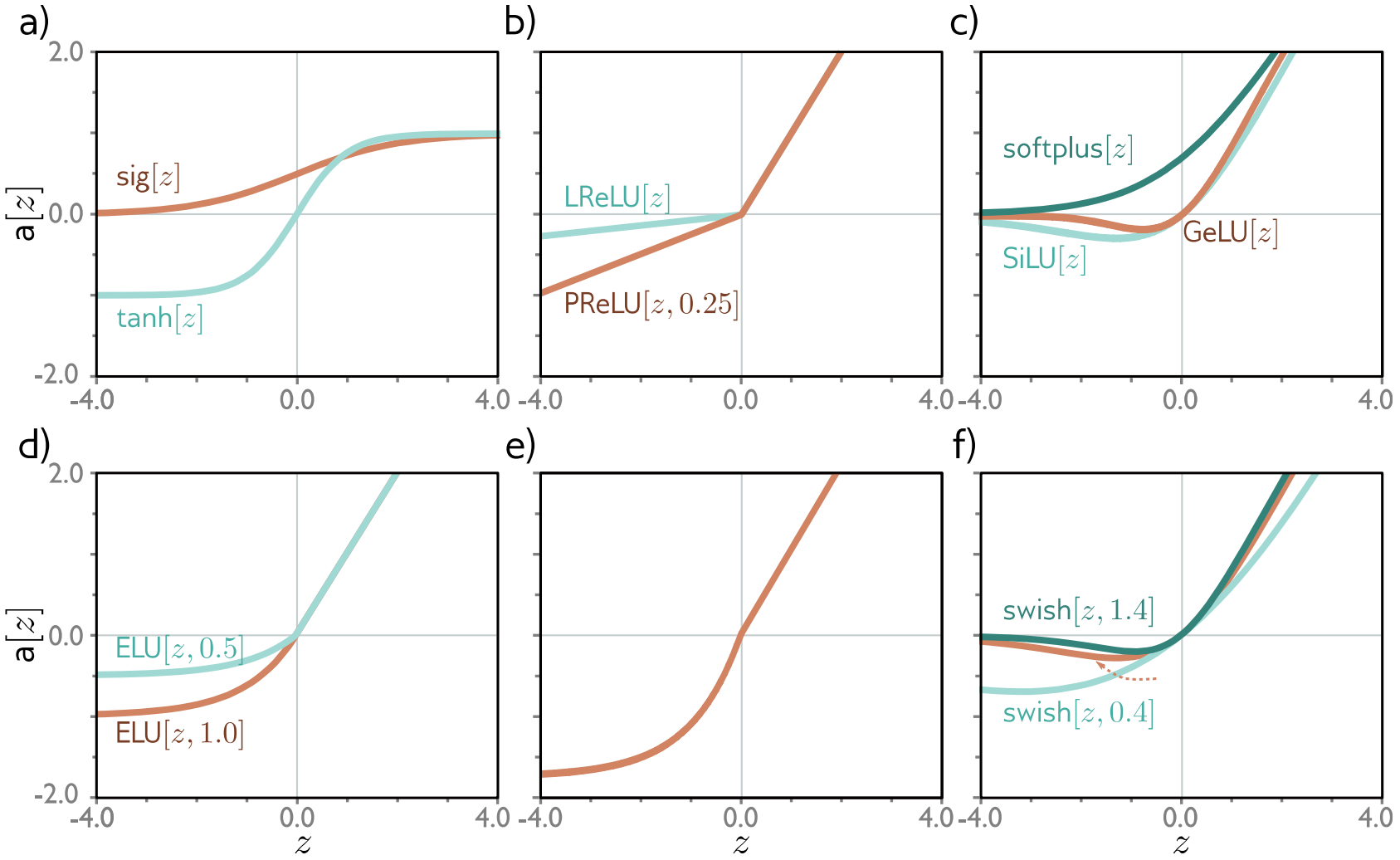
- D_o Outputs, D hidden units, and D_i inputs

$$h_d = \mathrm{a}\left[\theta_{d0} + \sum_{i=1}^{D_i} \theta_{di} x_i\right] \qquad y_j = \phi_{j0} + \sum_{d=1}^{D} \phi_{jd} h_d$$



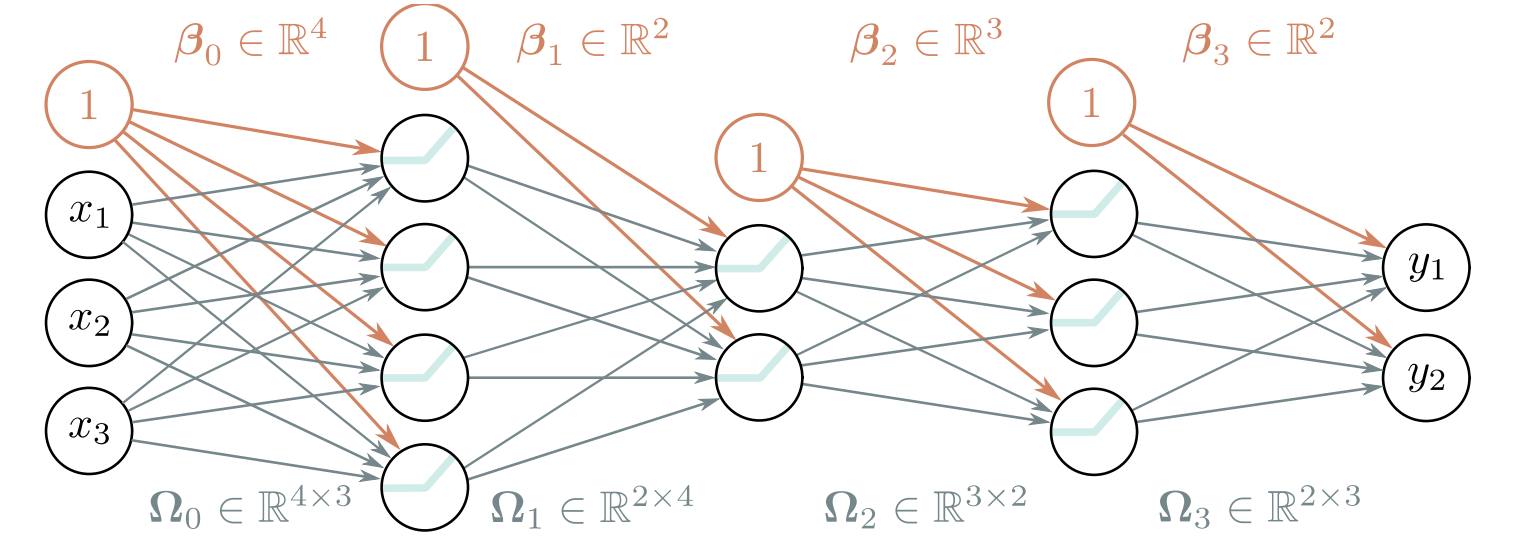
Activation functions

- Applied element-wise on their inputs
- Lead to non-linear models



Deep Neural Networks

- Deep neural networks
  - More flexible than shallow neural networks
  - Can have as many inputs and outputs as we want
  - Have *more than hidden layer* formed by as many units as we want



Shallow vs. Deep Neural Networks

The best results are created by deep networks with many layers.

- 10-1000 layers for most applications
- Best results in
  - Computer vision
  - Natural language processing
  - Graph neural networks
  - Generative models
  - Reinforcement learning

All use deep networks.
But why?

Shallow vs. Deep Neural Networks

1. Ability to approximate different functions?

Both obey the universal approximation theorem.

Argument: One layer is enough, and for deep networks could arrange for the other layers to compute the identity function.

Shallow vs. Deep Neural Networks

2. Depth efficiency

- There are some functions that require a shallow network with exponentially more hidden units than a deep network to achieve an equivalent approximation

- This is known as the depth efficiency of deep networks

- But do the real-world functions we want to approximate have this property? Unknown.

Shallow vs. Deep Neural Networks

3. Large structured networks

- Think about images as input – might be 1M pixels
- Fully connected works not practical
- Answer is to have weights that only operate locally, and share across image
- This leads to convolutional networks
- Gradually integrate information from across the image – needs multiple layers

Shallow vs. Deep Neural Networks

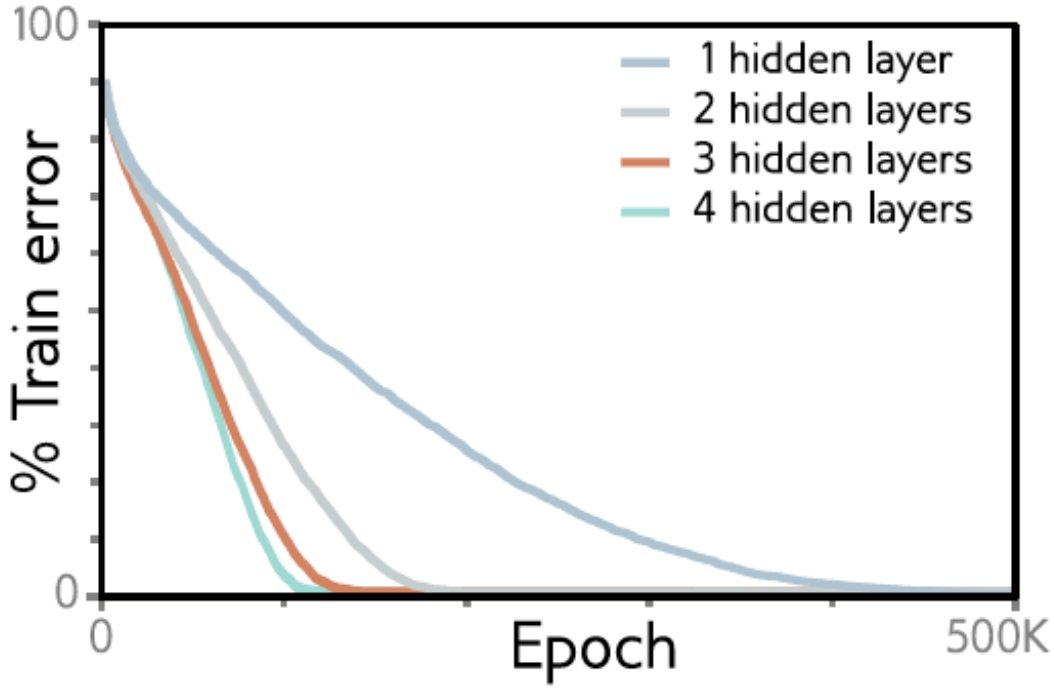
4. Fitting and generalization

- Fitting of deep models seems to be easier up to about 20 layers
- Then needs various tricks to train deeper networks, so (in vanilla form), fitting becomes harder
- Generalization is good in deep networks. Why?

Shallow vs. Deep Neural Networks

4. Fitting and generalization

Figure 20.2 MNIST-1D training. Four fully connected networks were fit to 4000 MNIST-1D examples with random labels using full batch gradient descent, He initialization, no momentum or regularization, and learning rate 0.0025. Models with 1,2,3,4 layers had 298, 100, 75, and 63 hidden units per layer and 15208, 15210, 15235, and 15139 parameters, respectively. All models train successfully, but deeper models require fewer epochs.



Training of neural networks

Model:

$$\mathbf{y} = \mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$$

- 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:

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

Parameters

Training of neural networks

Model:

$$\mathbf{y} = \mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$$

- Loss function:

$$L\left[\boldsymbol{\phi}\right]$$

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

- Find the parameters that minimize the loss:

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

Testing

- To test the model, run on a separate test dataset of input / output pairs

- See how well it generalizes to new data

How to construct loss functions

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

How to construct loss functions

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

How to construct loss functions

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

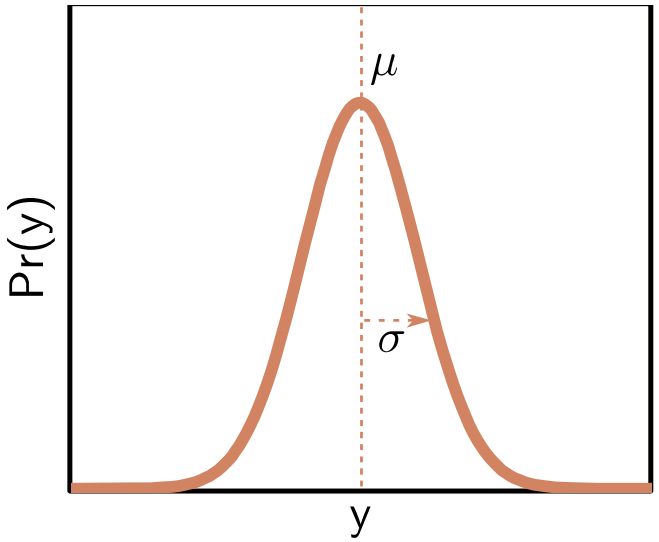
$$Pr(\mathbf{y}|\mathbf{x})$$

  over outputs **y** given inputs **x**.
- Loss function aims to make the outputs have high probability

How can a model predict a probability distribution?

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

Maximum likelihood criterion

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

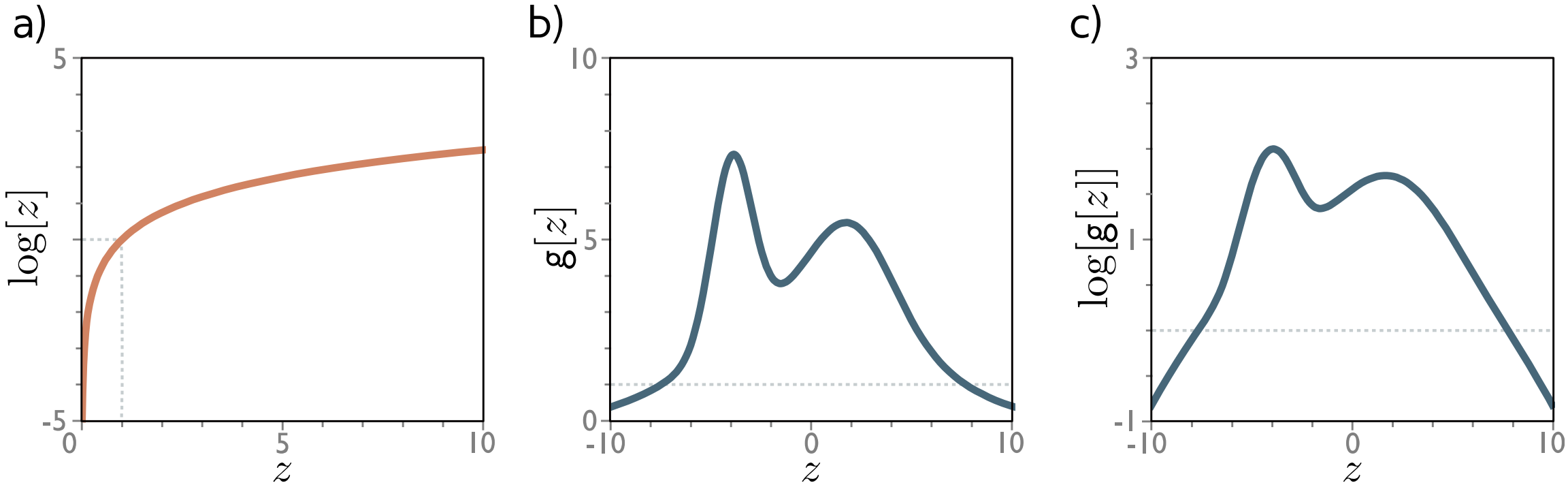
When we consider this probability as a function of the parameters $\boldsymbol{\phi}$, we call it a likelihood.

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

The log function is monotonic



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

Maximum log likelihood

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

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

Minimizing negative log likelihood

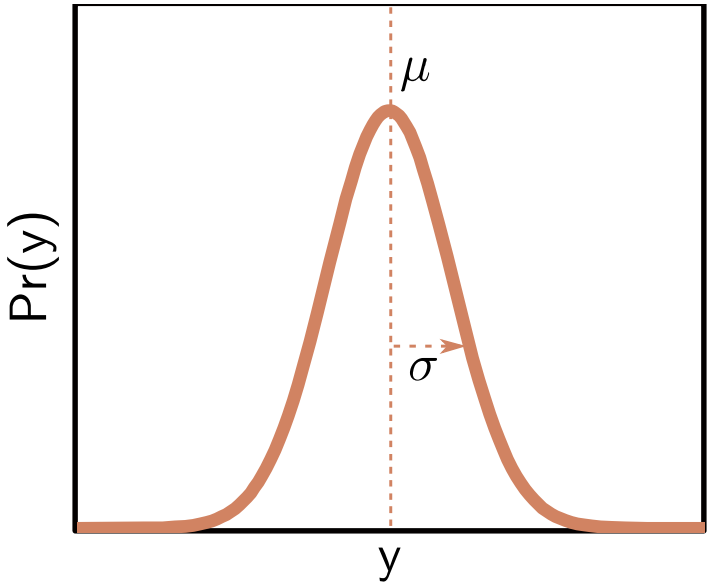
- By convention, we minimize things (i.e., a loss)

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

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)

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



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 $\boldsymbol{\theta}$.

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

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

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

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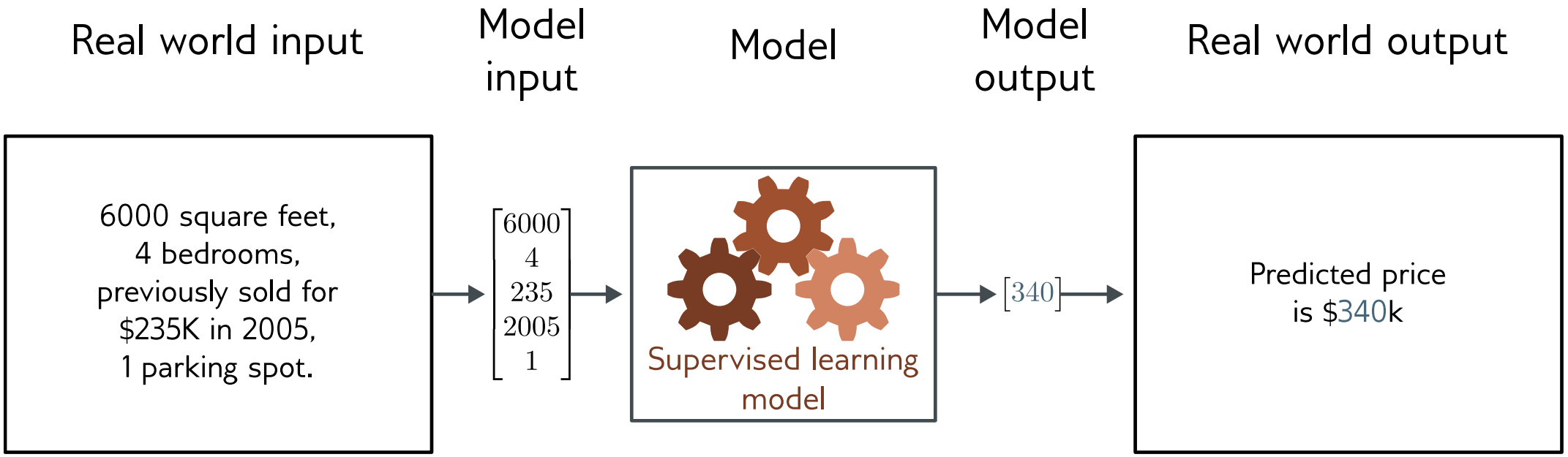
4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\boldsymbol{\phi}}])$ or the maximum of this distribution.

Example 1: univariate regression



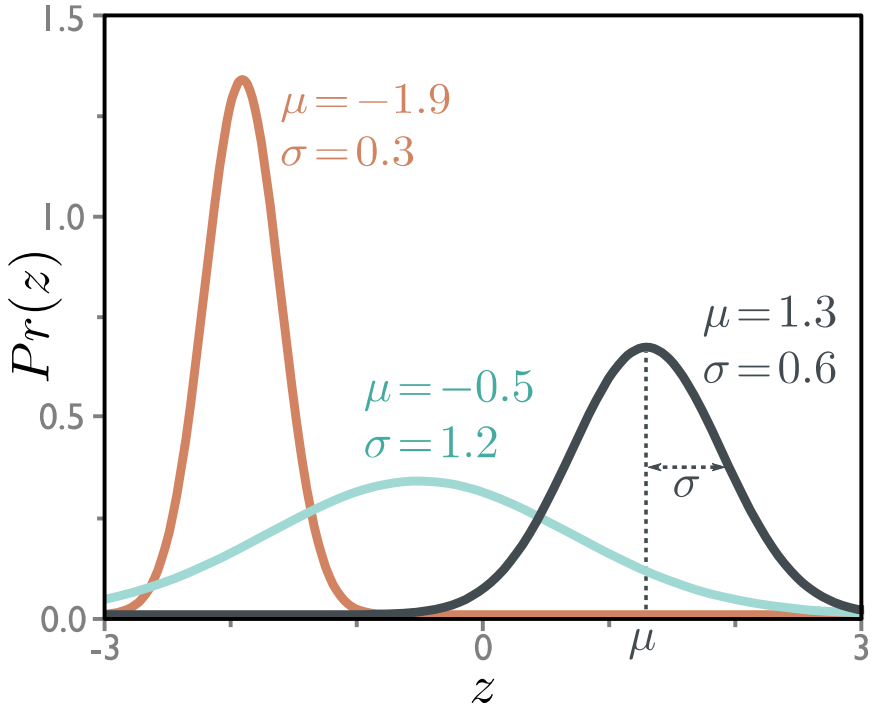
- Goal: predict the price y of a house described by x

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

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

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

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

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

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

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

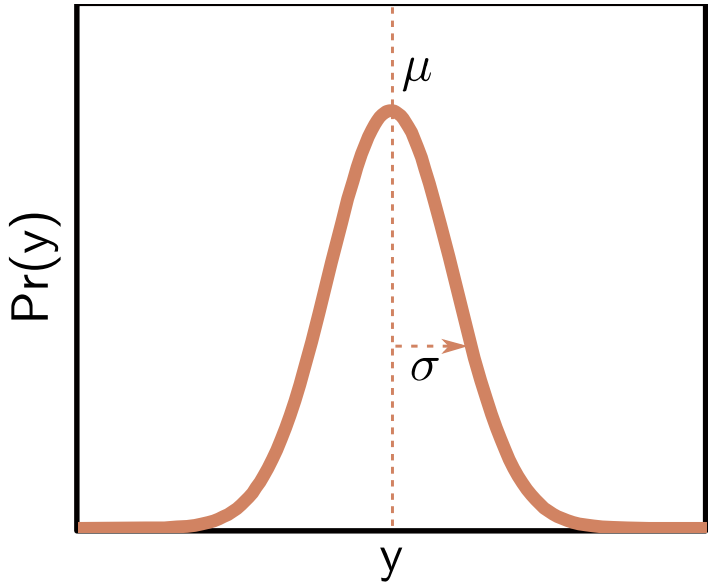
Least squares!

Example 1: univariate regression

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

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

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



Estimating variance

- Perhaps surprisingly, the variance term disappeared:

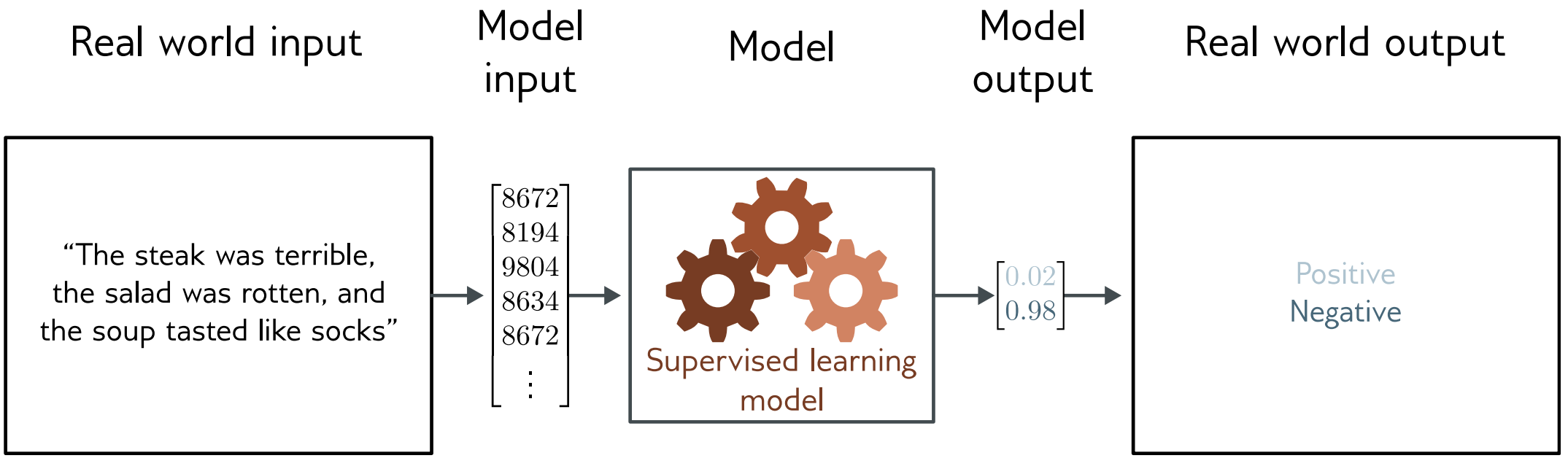
$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\sigma^2} \right] \right] \right]$$

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

- But we could learn it:

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

Example 2: binary classification



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

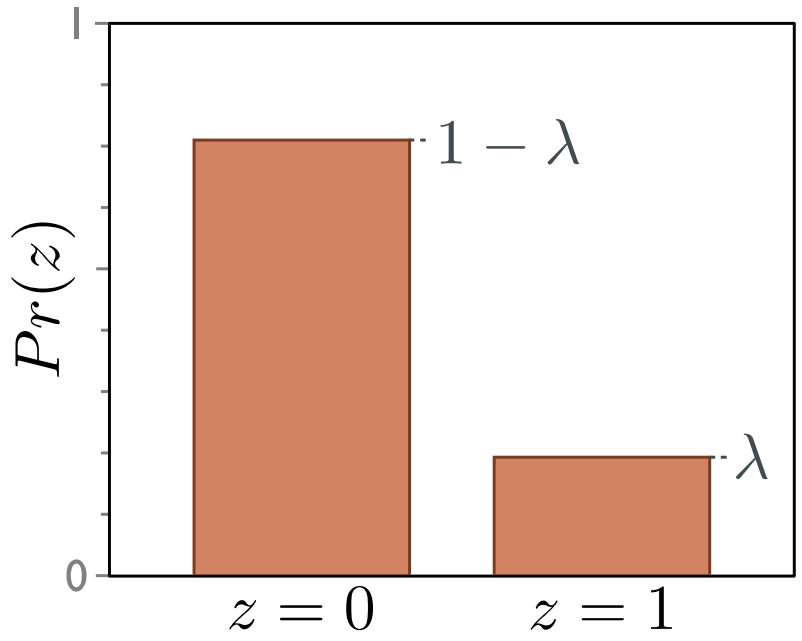
Example 2: binary classification

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 λ ∈[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 $\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$ 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 function that maps "anything" to [0,1]

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Problem:

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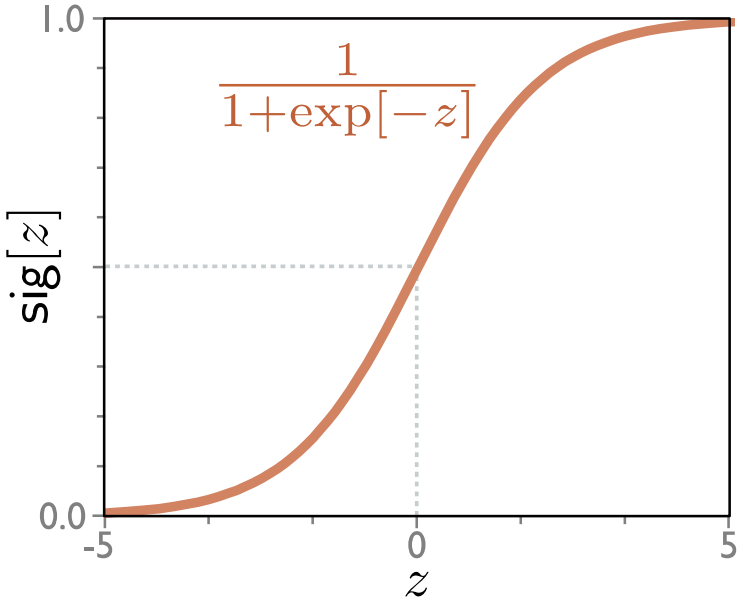
Solution:

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

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



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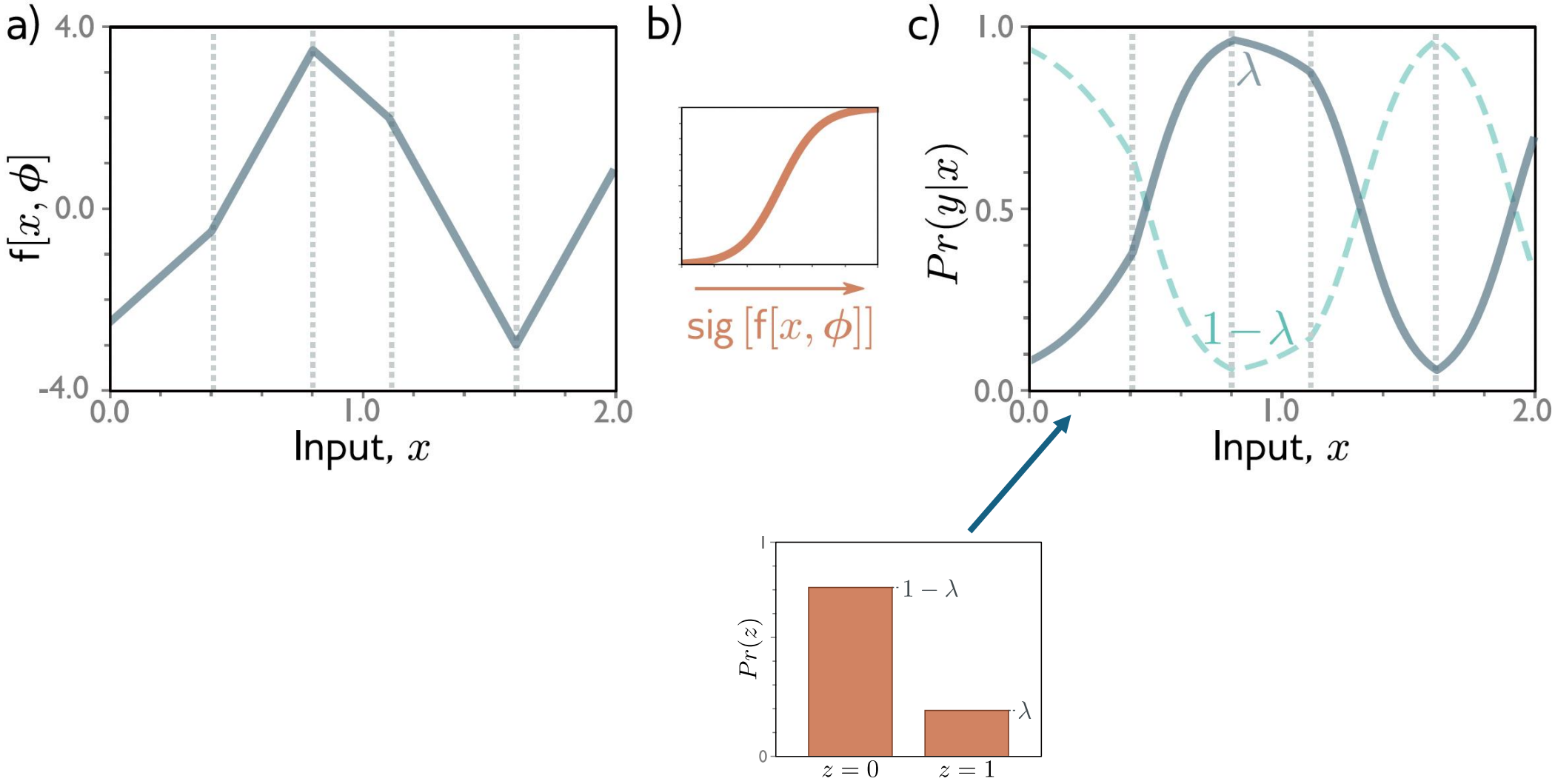
$$Pr(y|\lambda) = (1-\lambda)^{1-y} \cdot \lambda^{y}$$

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

Example 2: binary classification



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

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

Binary cross-entropy loss

Example 2: binary classification

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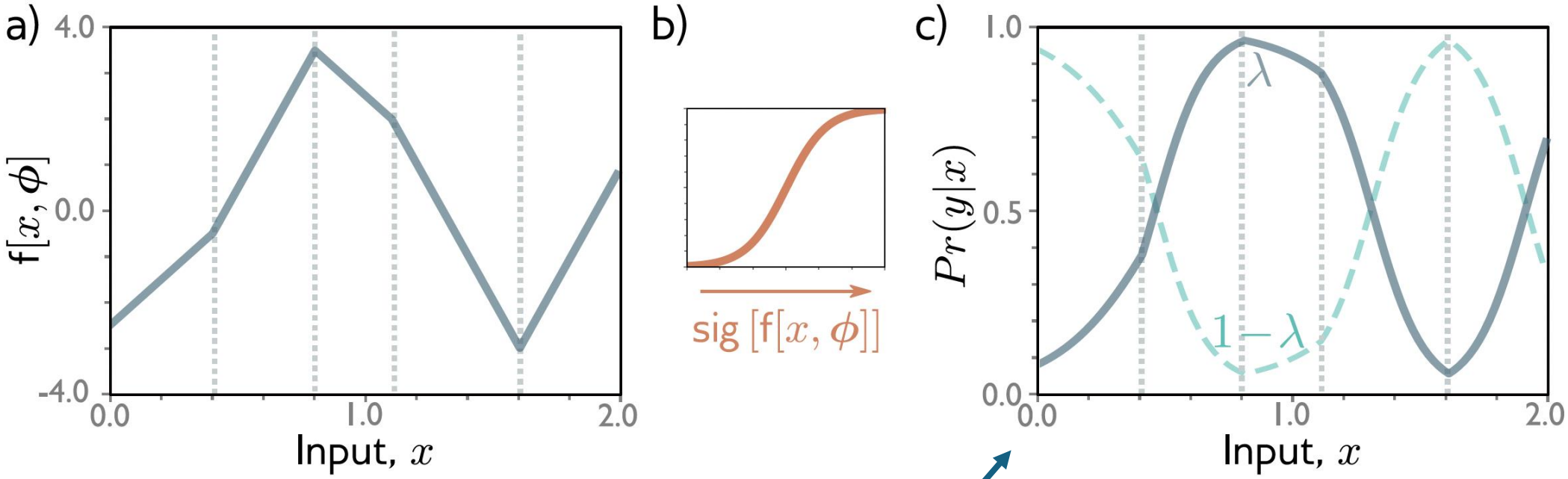
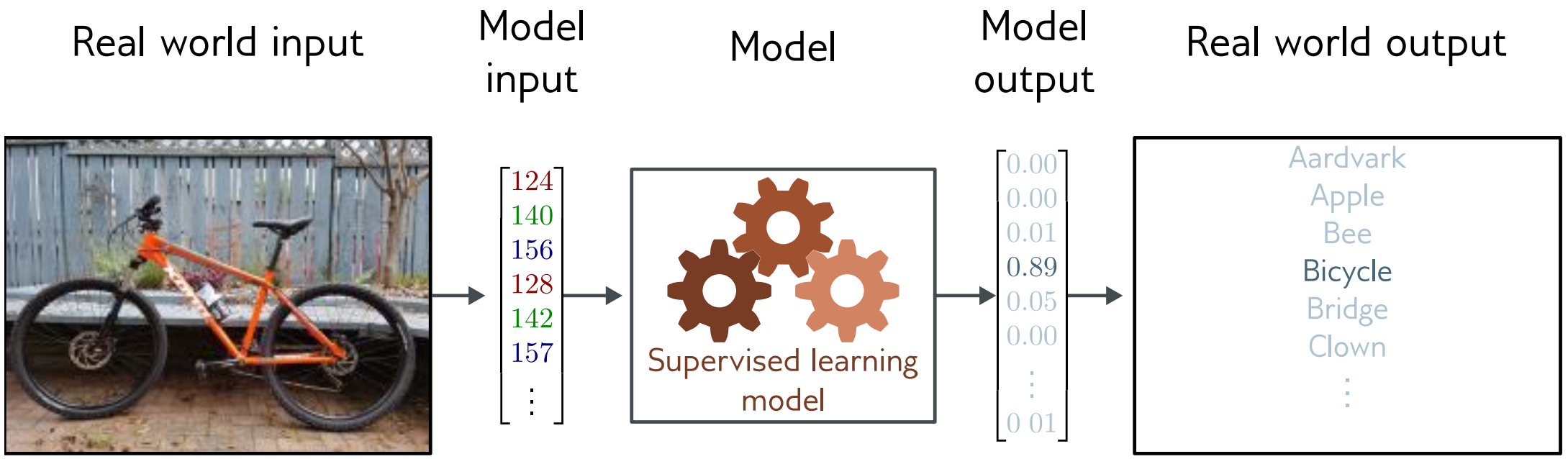


Choose y=1 where λ is greater than 0.5, otherwise 0

Example 3: multiclass classification



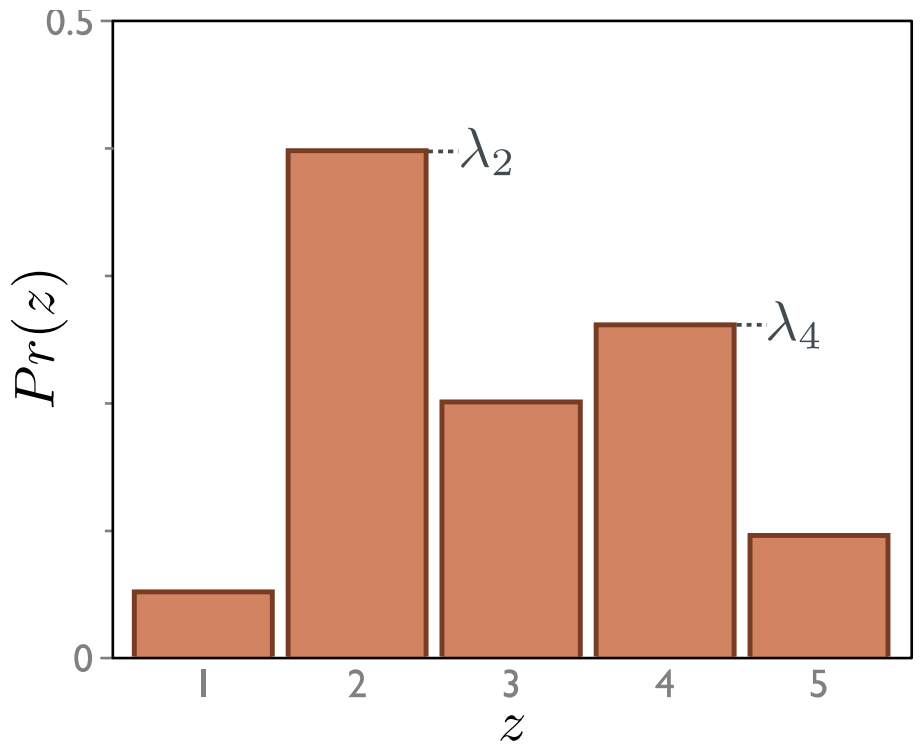
Goal: predict which of K classes $y \in \{1, 2, \ldots, K\}$ the input *x* belongs to

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 λ_k ∈[0,1]
- Sum of all parameters = 1

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



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Problem:

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

Solution:

- Pass through function that maps "anything" to [0,1], with sum of all outputs equal to one

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

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

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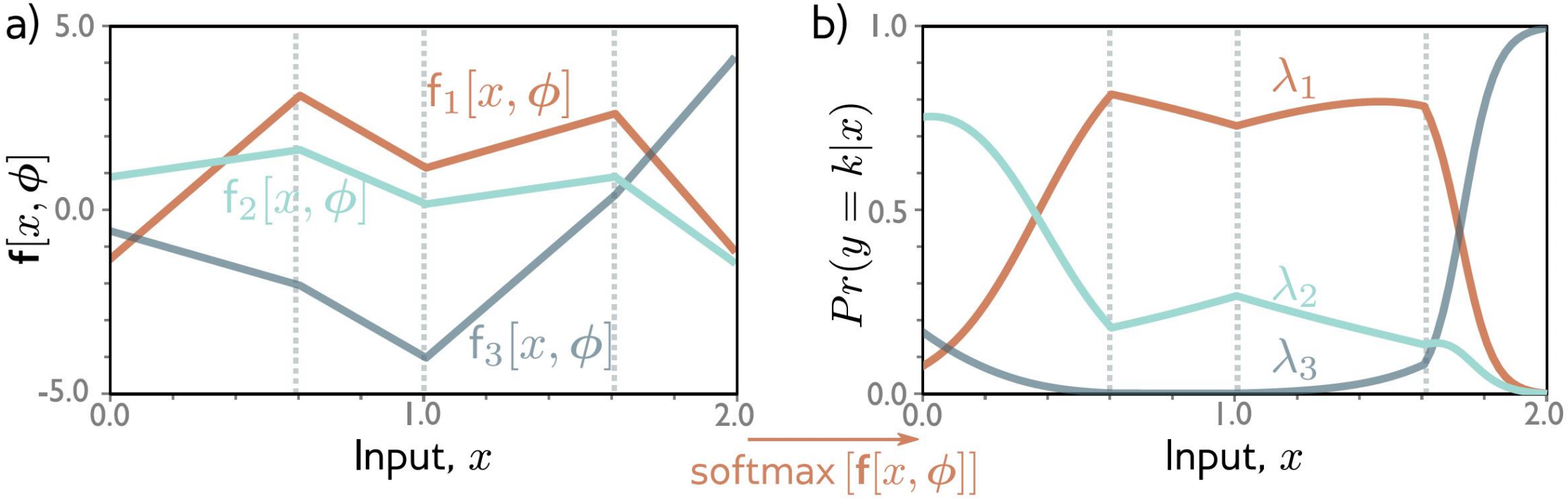


$$Pr(y = k|\mathbf{x}) = \mathrm{softmax}_k[\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]]$$

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

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

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

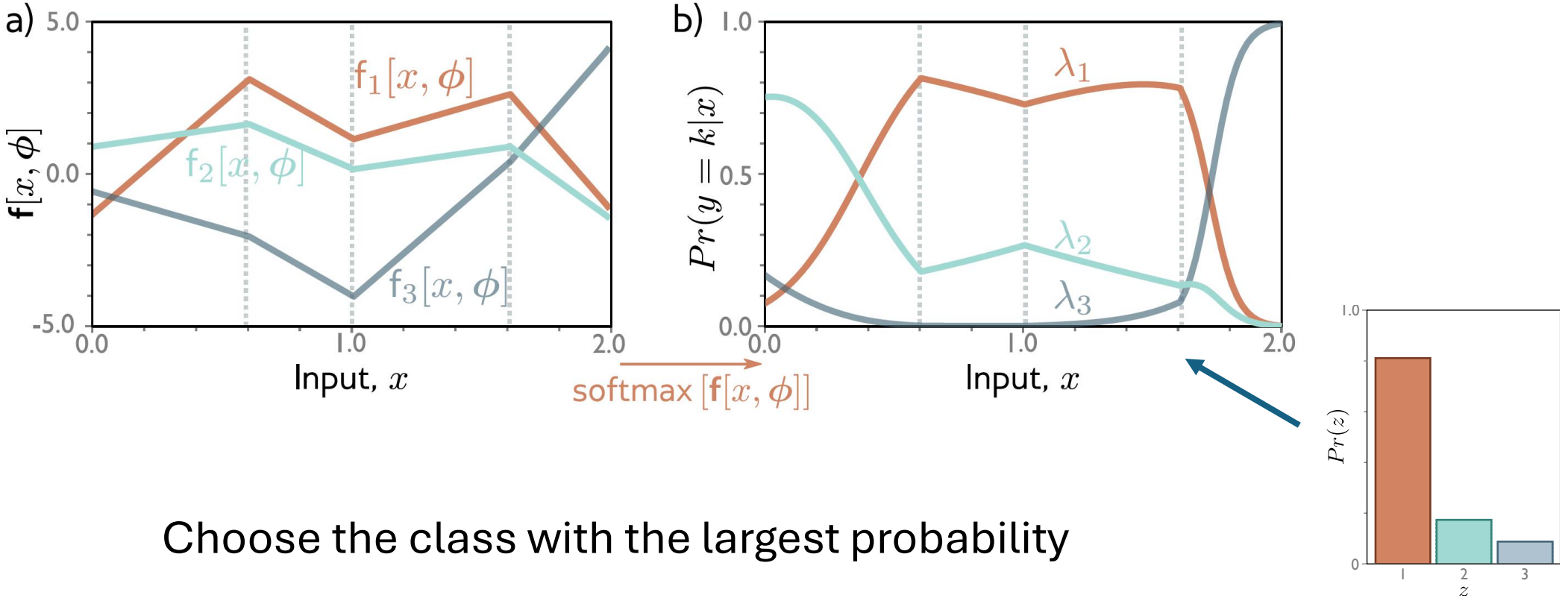
$$= -\sum_{i=1}^{I} \mathrm{f}_{y_i} \left[\mathbf{x}_i, \boldsymbol{\phi} \right] - \log \left[\sum_{k=1}^{K} \exp \left[\, \mathrm{f}_k \left[\mathbf{x}_i, \boldsymbol{\phi} \right] \right] \right]$$

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

Multiclass cross-entropy loss

Example 3: multiclass classification

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



Choose the class with the largest probability

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.

Multiple outputs

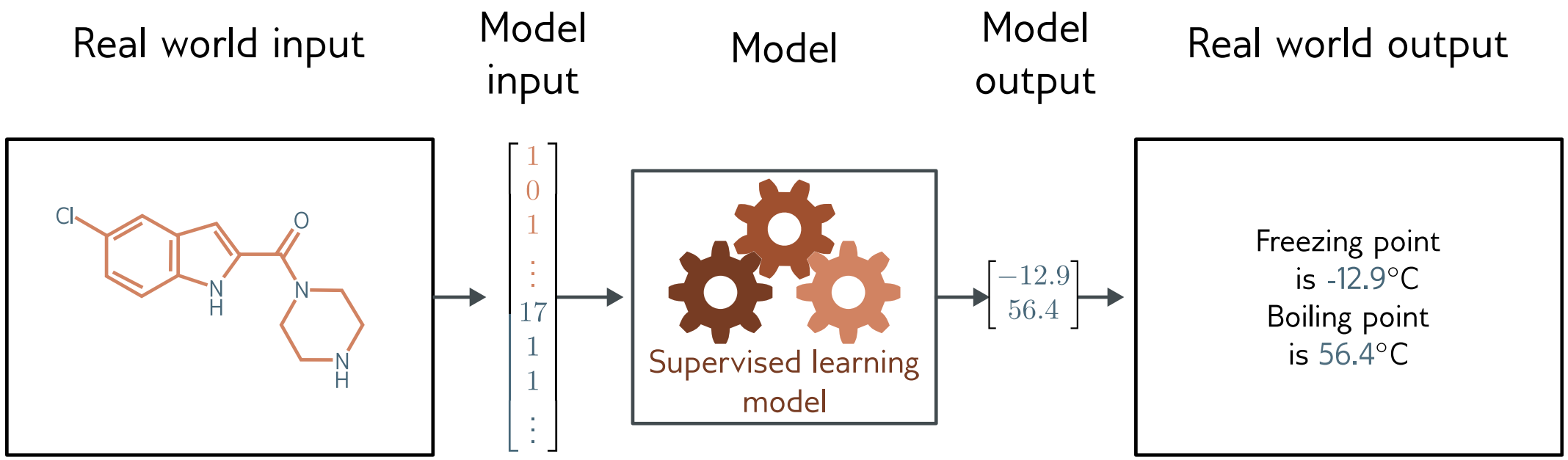
- Treat each output y_d as independent:

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

- Negative log likelihood becomes sum of terms:

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

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

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

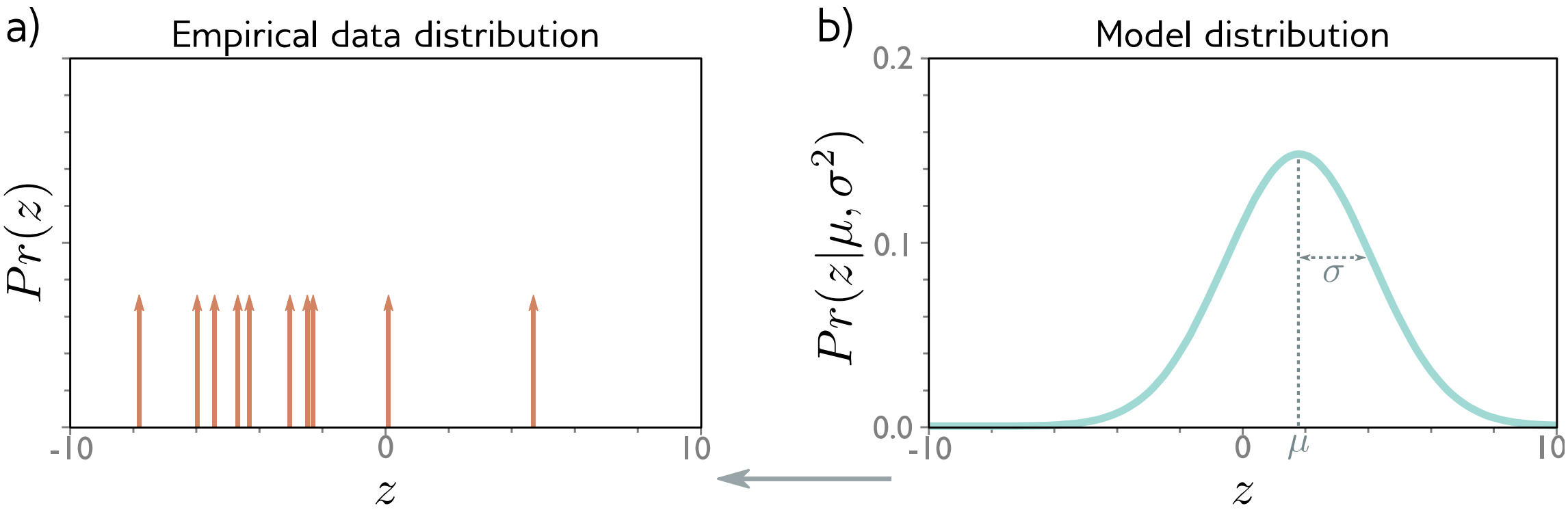
- Make a network with D_o outputs to predict means

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

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

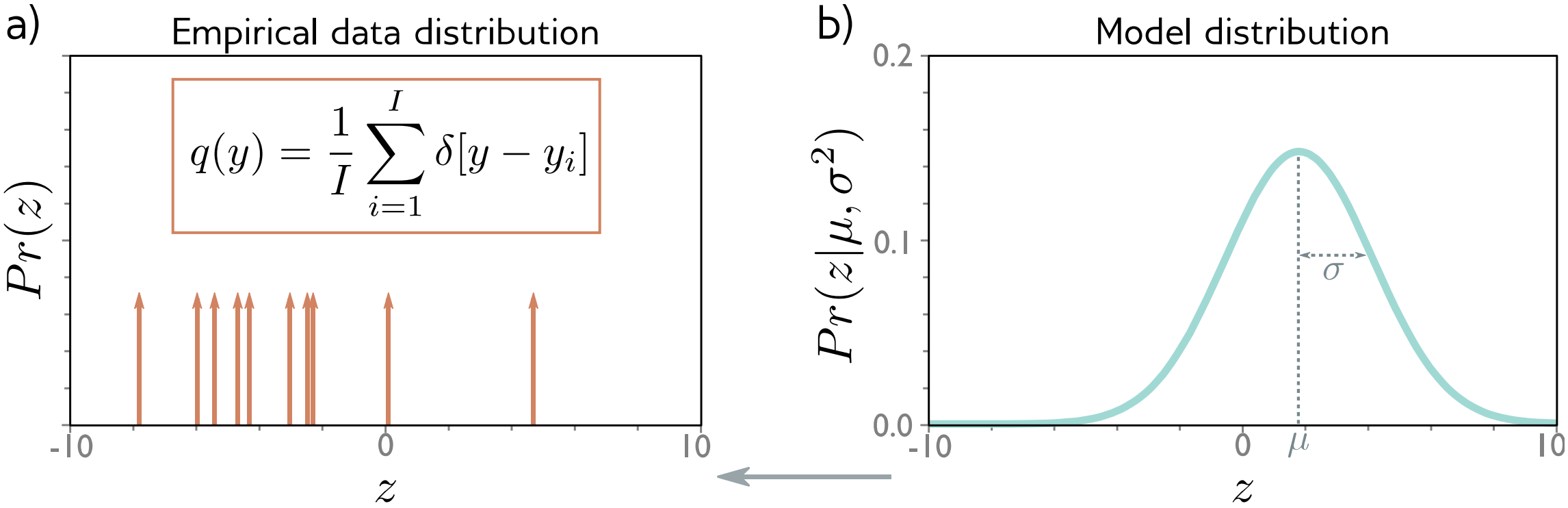
Cross Entropy



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

Kullback-Leibler Divergence -- a measure between probability distributions

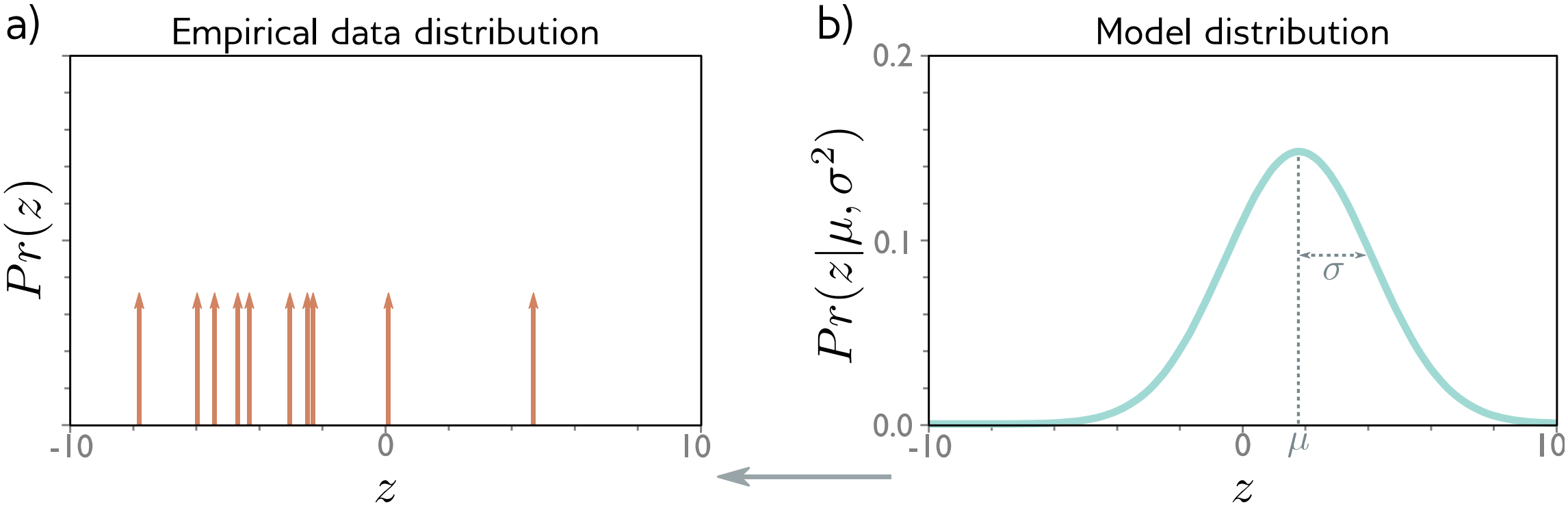
Cross Entropy



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

Kullback-Leibler Divergence -- a measure between probability distributions

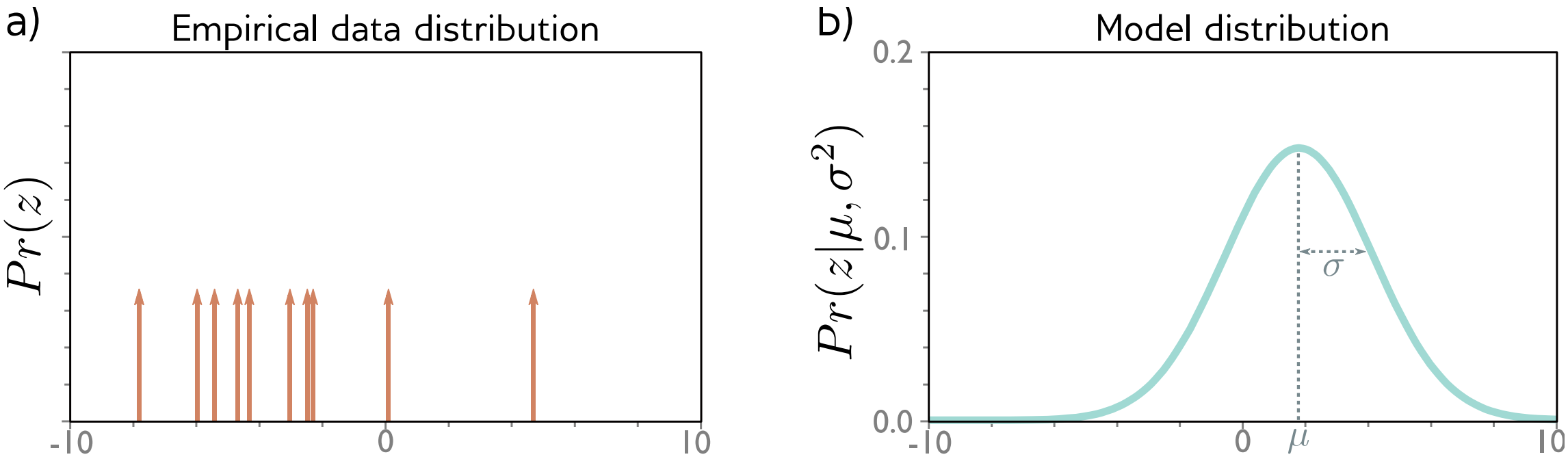
Cross Entropy



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

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

Cross Entropy



$$\hat{\boldsymbol{\theta}} = \underset{\theta}{\operatorname{argmin}} \left[-\int_{-\infty}^{\infty} \left(\frac{1}{I} \sum_{i=1}^{I} \delta[y - y_i] \right) \log \left[Pr(y|\boldsymbol{\theta}) \right] dy \right]$$

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

Minimum negative log likelihood