# Deep learning

Unpacking Transformers, LLMs and image generation

## Session 2

| Session | Lecture | Practical |
|---|---|---|
| 1 | Intro to DL<br>Gradient descent | • Micrograd |
| 2 | DL fundamentals I<br>• Backprop<br>• Loss functions<br>• Neural Probabilistic Language Model (Bengio 2003) | • Bigram model<br>• MLP for next-character prediction |
| 3 | DL fundamentals II<br>• Activation functions<br>• Regularization<br>• Initialization<br>• Residual networks<br>• Normalization<br>Recurrent neural networks | • Tensor-based MLP |
| 4 | Attention and Transformers | • GPT from scratch |
| 5 | DL for computer vision (convnets, u-nets) | • Convnets for CIFAR-10 |
| 6 | VAE & Diffusion models | • Diffusion from scratch |

# There is no reason for deep learning to work

**Training**: Finding the global optimum of an arbitrary non-convex function is NP-hard (Murty & Kabadi, 1987).

**Generalization**: deep networks generate way more regions than training samples.

# Neural networks generate large number of regions

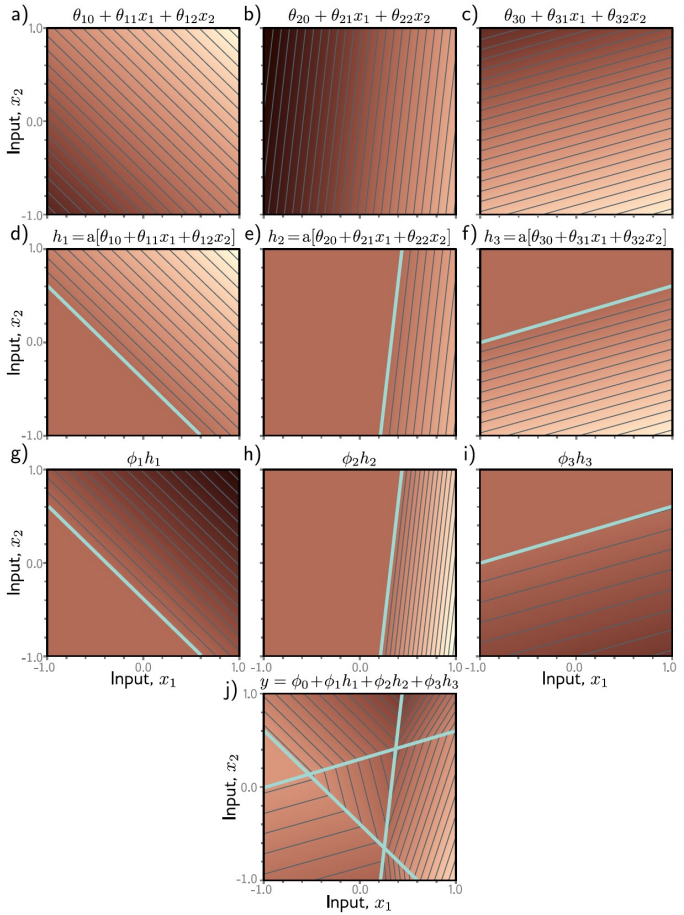



**Figure 3.8** Processing in network with two inputs $\mathbf{x} = [x_1, x_2]^T$, three hidden units $h_1, h_2, h_3$, and one output $y$. a–c) The input to each hidden unit is a linear function of the two inputs, which corresponds to an oriented plane. Brightness indicates function output. For example, in panel (a), the brightness represents $\theta_{10} + \theta_{11}x_1 + \theta_{12}x_2$. Thin lines are contours. d–f) Each plane is clipped by the ReLU activation function (cyan lines are equivalent to "joints" in figures 3.3d–f). g-i) The clipped planes are then weighted, and j) summed together with an offset that determines the overall height of the surface. The result is a continuous surface made up of convex piecewise linear polygonal regions.

A neural network generate a number of linear sub-regions.

Source: Understanding Deep Learning, S. Prince, 2023

# Shallow networks generate large number of regions

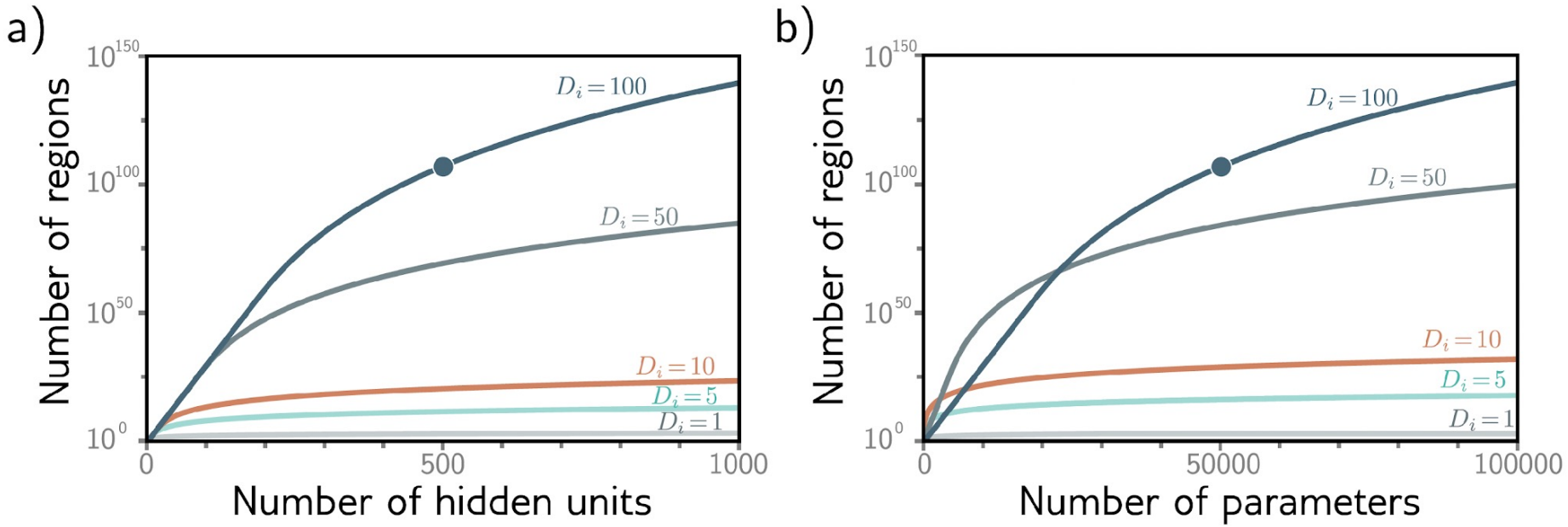



**Figure 3.9** Linear regions vs. hidden units. a) Maximum possible regions as a function of the number of hidden units for five different input dimensions $D_i = \{1, 5, 10, 50, 100\}$. The number of regions increases rapidly in high dimensions; with $D = 500$ units and input size $D_i = 100$, there can be greater than $10^{107}$ regions (solid circle). b) The same data are plotted as a function of the number of parameters. The solid circle represents the same model as in panel (a) with $D = 500$ hidden units. This network has $51,001$ parameters and would be considered very small by modern standards.

Source: Understanding Deep Learning, S. Prince, 2023

# Deep networks generate even more of regions / parameter count

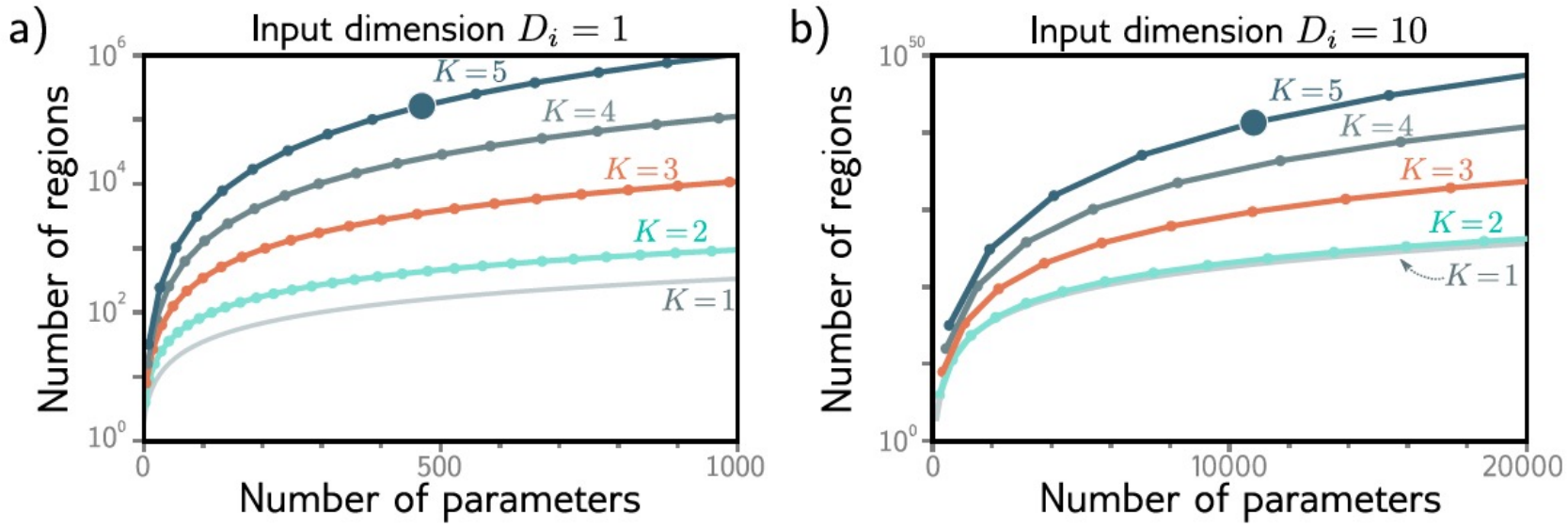



**Figure 4.7** The maximum number of linear regions for neural networks increases rapidly with the network depth. a) Network with $D_i = 1$ input. Each curve represents a fixed number of hidden layers $K$, as we vary the number of hidden units $D$ per layer. For a fixed parameter budget (horizontal position), deeper networks produce more linear regions than shallower ones. A network with $K = 5$ layers and $D = 10$ hidden units per layer has 471 parameters (highlighted point) and can produce 161,051 regions. b) Network with $D_i = 10$ inputs. Each subsequent point along a curve represents ten hidden units. Here, a model with $K = 5$ layers and $D = 50$ hidden units per layer has 10,801 parameters (highlighted point) and can create more than $10^{40}$ linear regions.

Source: Understanding Deep Learning, S. Prince, 2023

# Deep networks generate even more of regions / parameter count

The number of regions grows exponentially with the depth of the network but only polynomial with the width of the hidden layers [1].

→ Deep neural networks create much more complex functions for a fixed parameter budget.

[1] On the number of linear regions of deep neural networks, Montufar et al, NeurIPS 2014.

# Deep networks generate even more of regions / parameter count

Deep neural networks create much more complex functions for a fixed parameter budget.

With 1D input, 1D output, D hidden units:

| | # regions | # parameters |
|---|---|---|
| Shallow network | $D+1$ | $3D+1$ |
| Deep network (K layers) | $(D+1)^K$ | $3D+1+(K-1)D(D+1)$ |

# Let’s venture into the variations of a deep networks

Network architecture and inductive bias

Loss function

Activation function

Regularization

Initialization

Residual networks

Batch norm, layer norm

# Inductive bias

Set of assumptions made by the model about the relationship between input data and output data.

Examples:

- Minimum features
- Maximum margin (SVM)
- Minimum cross-validation error
- Neural net architecture (convnet, transformer)

# Do networks have to be deep?

Empirical evidence: shallow networks don’t work as well as deeper ones.

Intuition:

1. Deep networks can represent more complex functions with the parameter count
2. Deep networks are easier to train
3. Deep network impose better inductive bias

# The challenges of depth

- Vanishing/exploding gradients
- Shattered gradients

In short, depth is required but comes with challenges that need to be addressed.

# Let’s venture into the variations of a deep networks

Network architecture and inductive bias

Loss function

Activation function

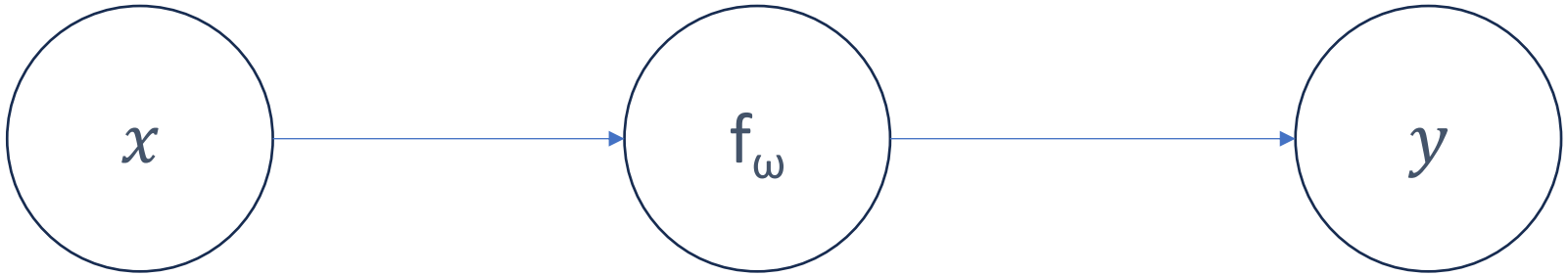
Regularization

Initialization

Residual networks

Batch norm, layer norm

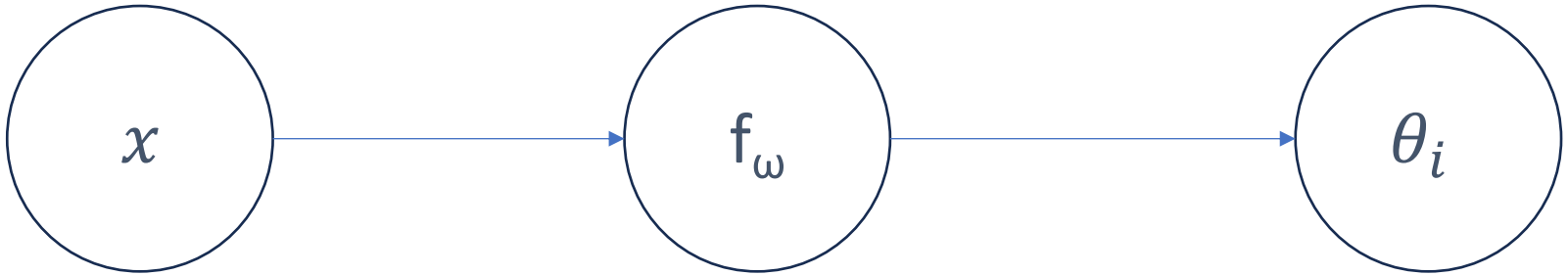
# Loss functions




$$\ell = (y - \hat{y})^2$$

ground-truth

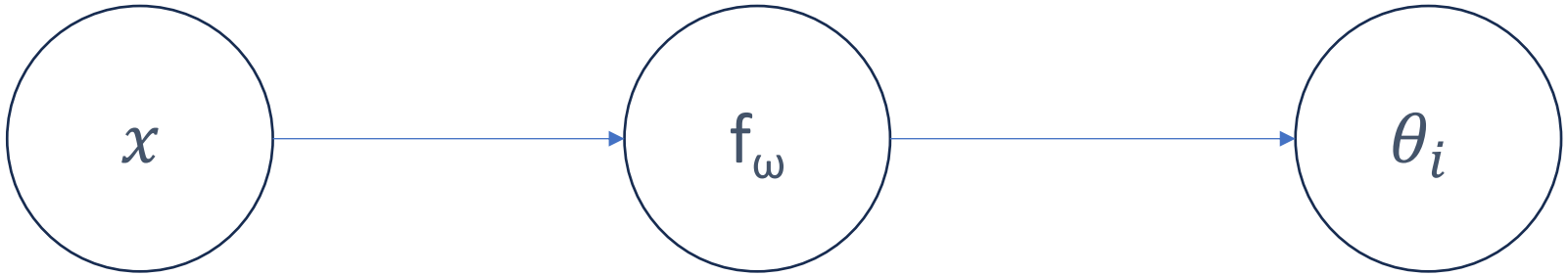
# Loss functions




$$f_\omega(x_i) = \theta_i$$

Parameters of a distribution

# Loss functions



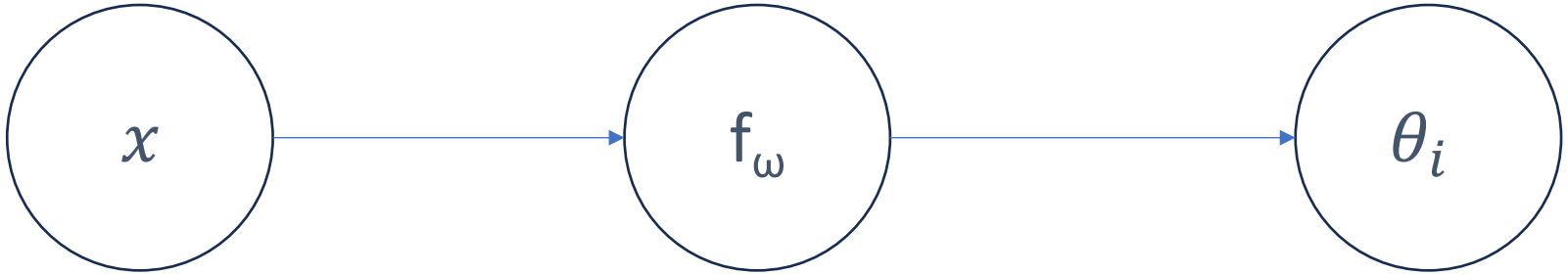

$$f_\omega(x_i) = \theta_i$$

The distribution is chosen based on the domain.

The model computes the optimal $\theta_i$ given the data.

# Loss functions

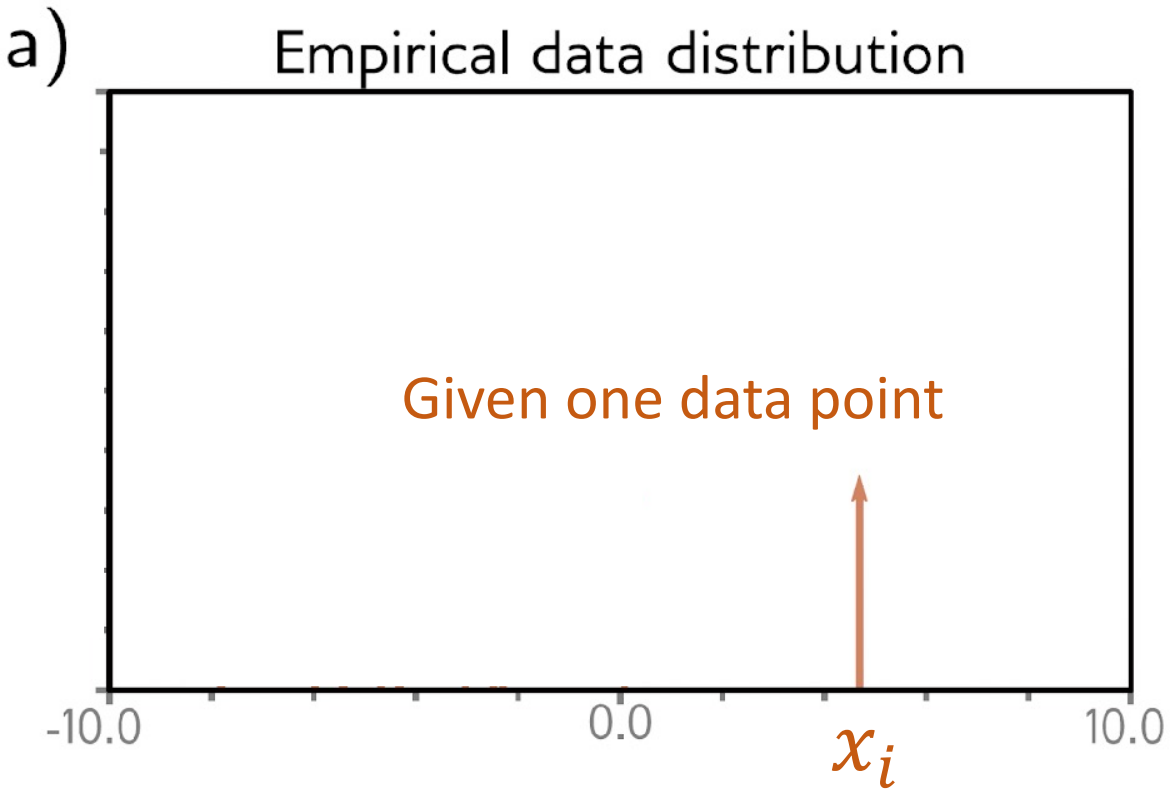
$$f_\omega(x_i) = \theta_i$$

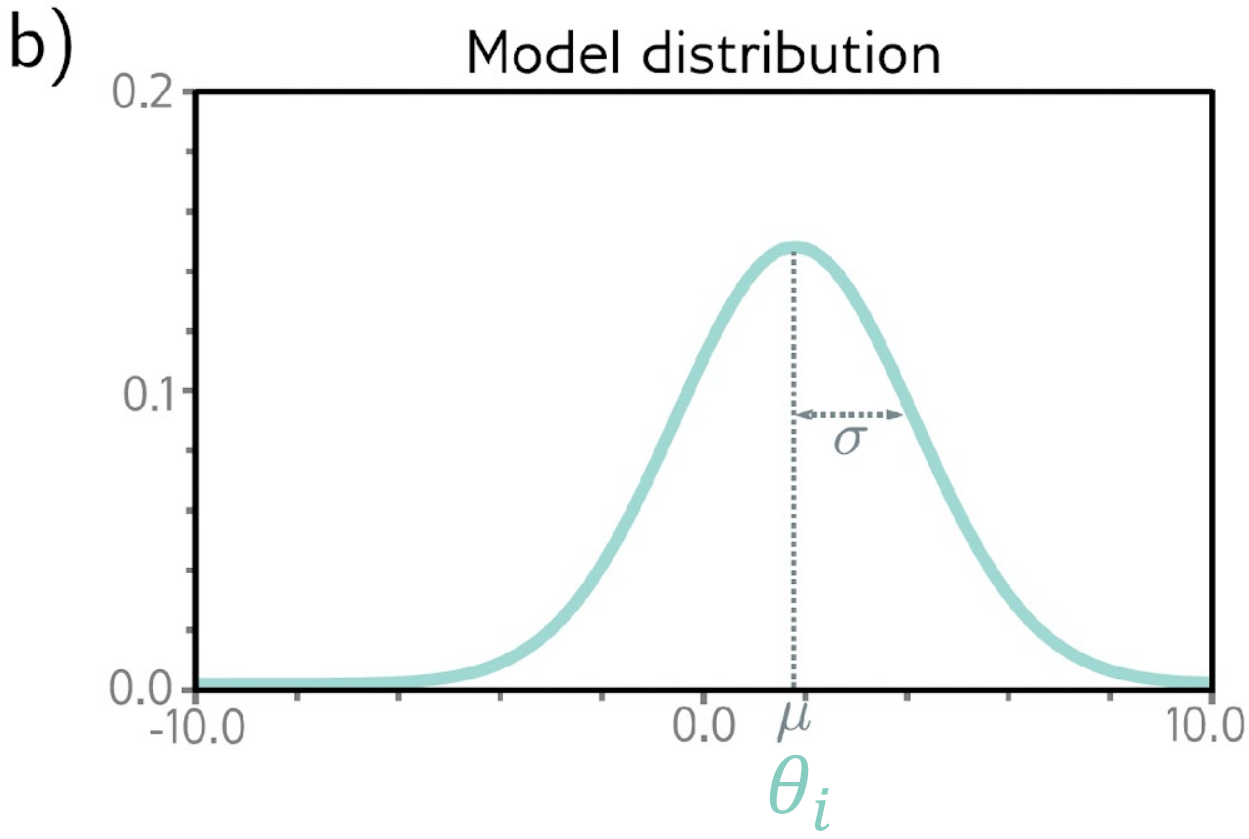



Example: univariate regression

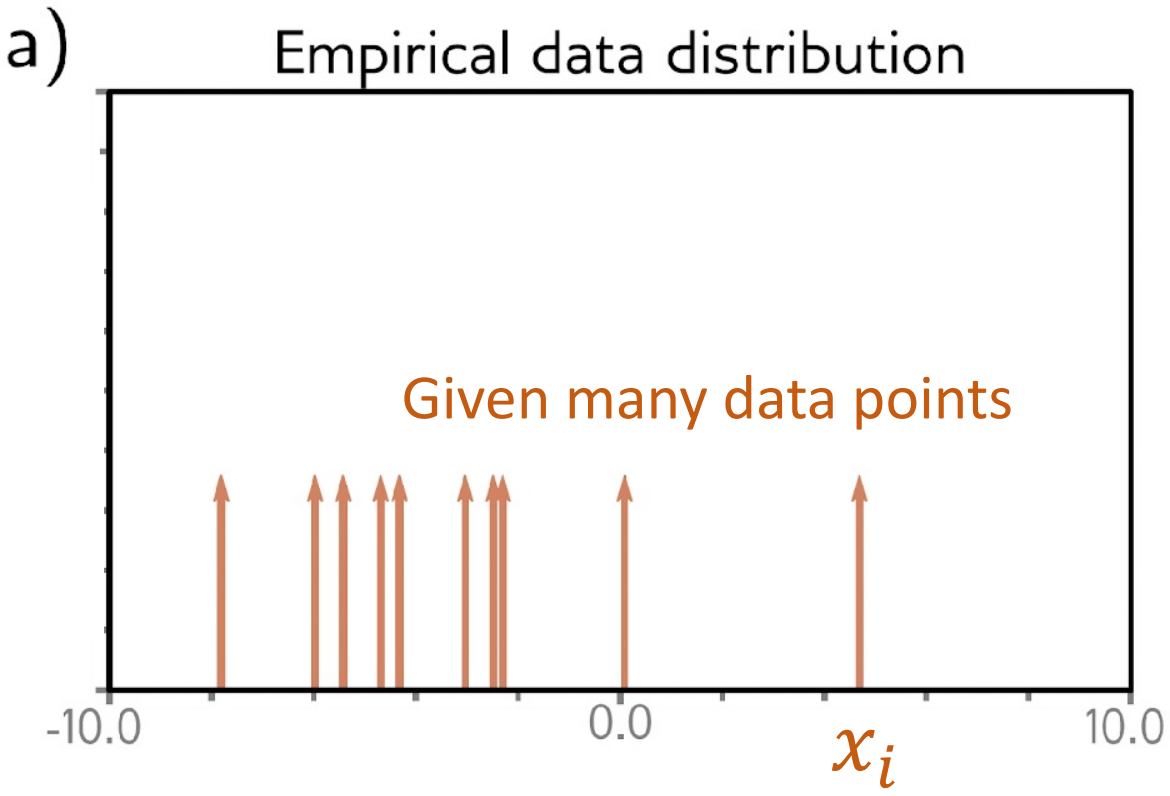
$$\Pr(y|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

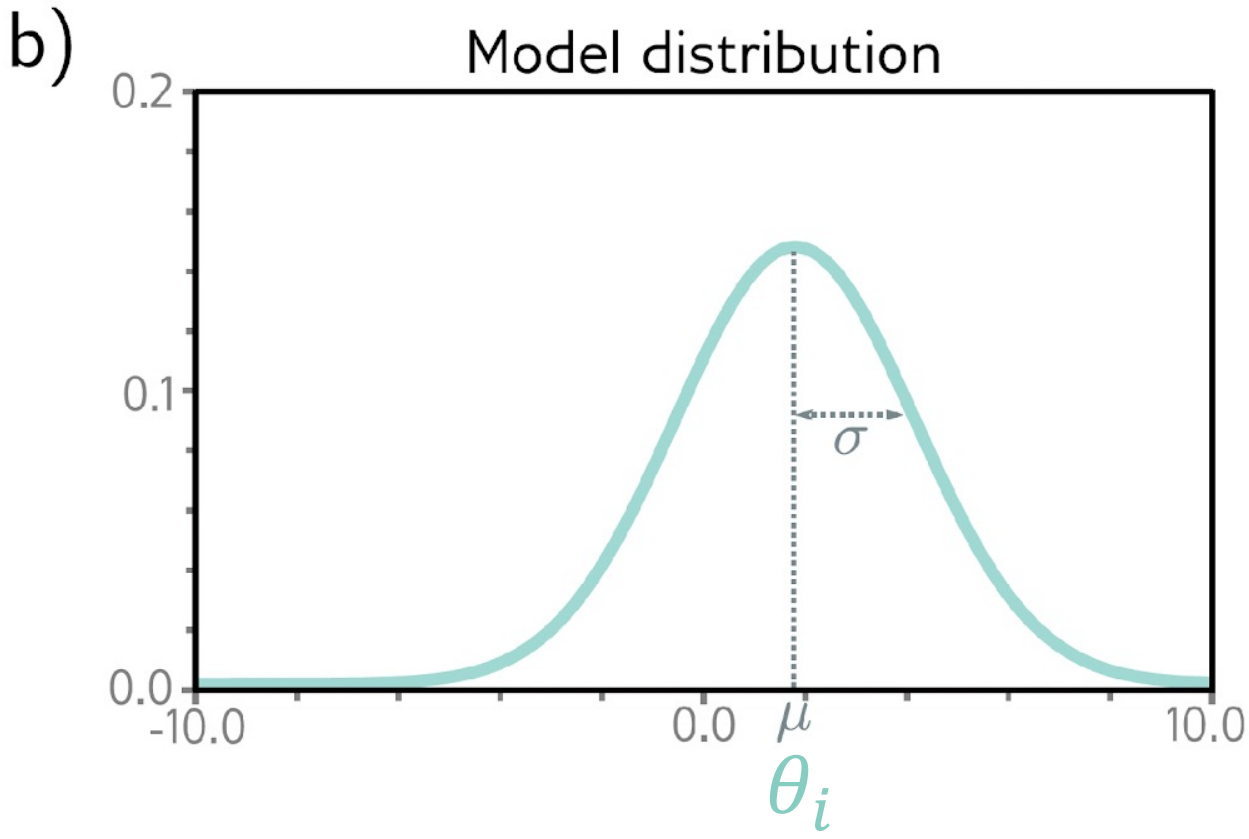
$\theta$




Predict the corresponding distribution parameter




Predict the corresponding distribution parameters

$$f_\omega(x_i) = \theta_i$$

# Loss functions

$$\hat{\omega} = \underset{\omega}{\operatorname{argmax}} \left[ \prod_{i=1}^{N} \Pr(y_i | x_i) \right]$$

$$= \underset{\omega}{\operatorname{argmax}} \left[ \prod_{i=1}^{N} \Pr(y_i | \theta_i) \right]$$

$$= \underset{\omega}{\operatorname{argmax}} \left[ \prod_{i=1}^{N} \Pr(y_i | f_\omega(x_i)) \right]$$

# Loss functions

$$\Pr(y_1, y_2, \ldots, y_N | x_1, x_2, \ldots, x_N)$$

Data is assumed i.i.d

$$\hat{\omega} = \underset{\omega}{\operatorname{argmax}} \left[ \prod_{i=1}^{N} \Pr(y_i | x_i) \right]$$

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$$= \underset{\omega}{\text{argmax}} \left[ \prod_{i=1}^{N} \Pr(y_i|f_\omega(x_i)) \right]$$

$$= \underset{\omega}{\text{argmax}} \left[ \sum_{i=1}^{N} \log[\Pr(y_i|f_\omega(x_i))] \right]$$

$$= \underset{\omega}{\text{argmin}} \left[ -\sum_{i=1}^{N} \log[\Pr(y_i|f_\omega(x_i))] \right]$$

*Negative log likelihood (NLL)*

# Inference

Given new input data

$$\hat{y} = \underset{\omega}{\text{argmax}}[\Pr(y|f_\omega(x)]$$

Optimal choice: maximum of the distribution

Or sample from the distribution!

# Loss functions

In the case of the univariate regression, the NLL is equivalent to least squares.

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ -\sum_{i=1}^{N} \log[\Pr(y_i | f_\omega(x_i))] \right]$$

Negative log likelihood (NLL)

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ -\sum_{i=1}^{N} \log \left[ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-\mu)^2}{2\sigma^2}} \right] \right]$$

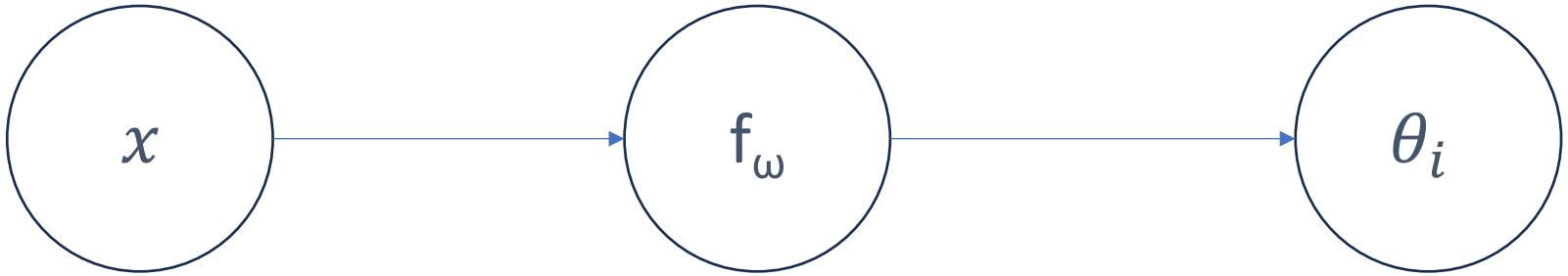
$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ -\sum_{i=1}^{N} \log \left[ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-f_\omega(x_i))^2}{2\sigma^2}} \right] \right]$$

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ \sum_{i=1}^{N} (y_i - f_\omega(x_i))^2 \right]$$

least squares

# Loss functions

$$f_\omega(x_i) = \theta_i$$



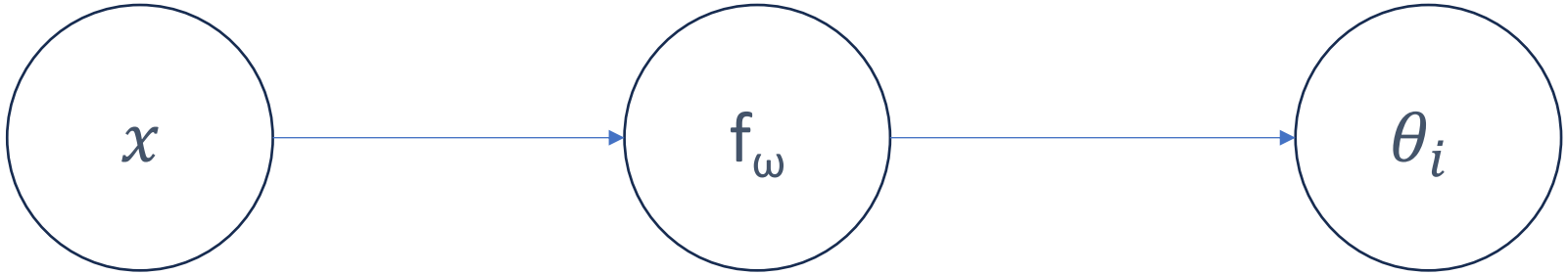

Example: binary classification

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

$\theta$

# Loss functions

$$f_\omega(x_i) = \theta_i$$




Example: binary classification

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

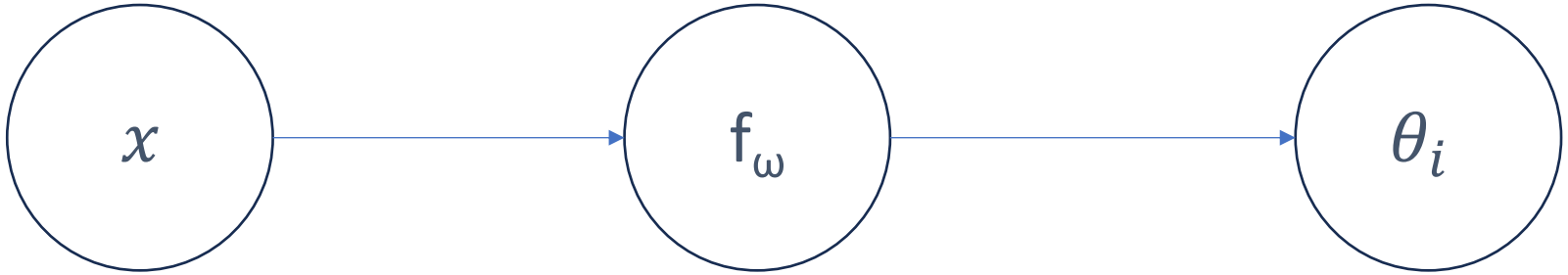
NLL

$$\ell = \sum_{i=1}^{N} -(1-y_i)\log[1-\sigma(f_\omega(x_i))] - y_i \log[\sigma(f_\omega(x_i))]$$

$\sigma$: sigmoid function

# Loss functions

$$f_\omega(x_i) = \theta_i$$



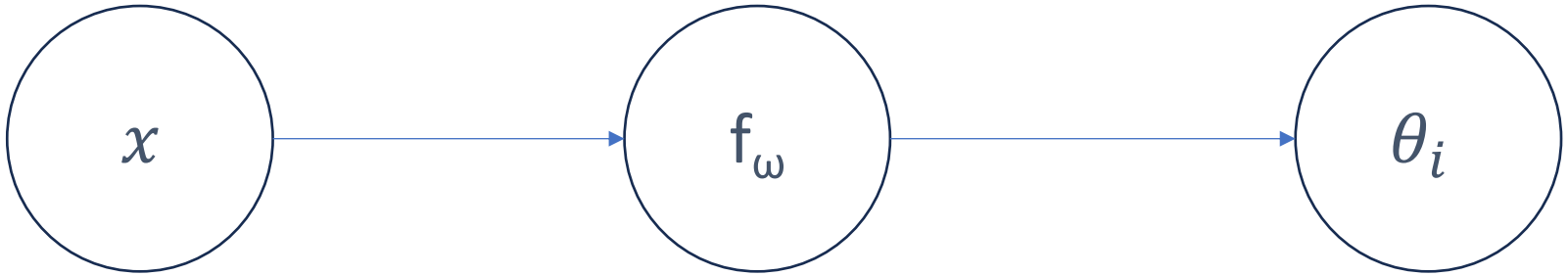

Example: multiclass classification

$$\Pr(y = k) = \lambda_k \qquad \sum \lambda_k = 1 \qquad 0 < \lambda_k < 1$$

$$\Pr\big((y = k|x)\big) = softmax_k[f_\omega(x)] \qquad softmax(\boldsymbol{z}) = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

# Loss functions

$$f_\omega(x_i) = \theta_i$$




Example: multiclass classification

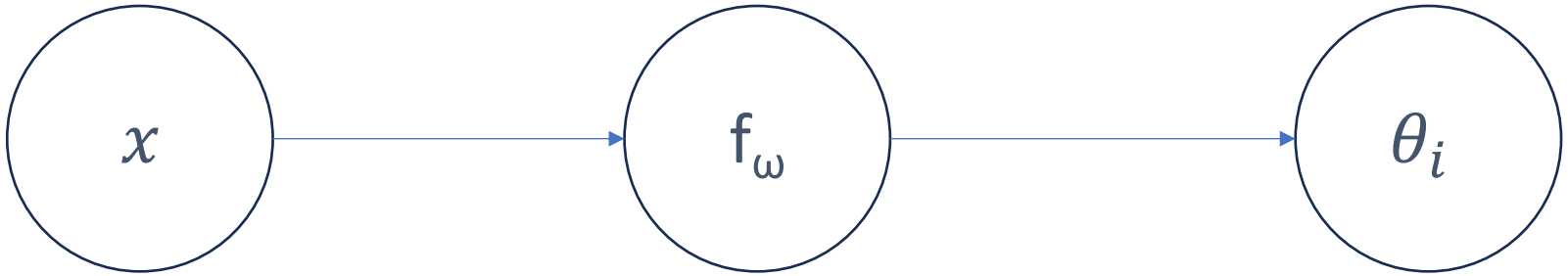
$$\Pr(y = k) = \lambda_k \qquad \sum \lambda_k = 1$$

NLL

$$\ell = -\sum_{i=1}^{N} \log\left[softmax_{y_i}[f_\omega(x_i)]\right]$$

# Loss functions

$$f_\omega(x_i) = \theta_i$$




Example: multiclass classification

$$\Pr(y = k) = \lambda_k \qquad \sum \lambda_k = 1$$

Wait, can I differentiate softmax?

NLL

$$\ell = -\sum_{i=1}^{N} \log\left[softmax_{y_i}[f_\omega(x_i)]\right]$$

Yes, and you will do it by hand in TP3!

# Loss functions

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ -\sum_{i=1}^{N} \log[\Pr(y_i | f_\omega(x_i))] \right]$$

Negative log likelihood (NLL)

is equivalent to the cross-entropy loss

# Loss functions

Given two distributions $q(z)$ and p$(z)$, the distance between the two distributions can be computed with:

$$D_{KL}(q|p) = \int_{-\infty}^{\infty} q(z)\log\big(q(z)\big)\,dz - \int_{-\infty}^{\infty} q(z)\log\big(p(z)\big)\,dz$$

Given an empirical distribution $q(y)$ and a model distribution $Pr(y|\omega)$, we want to minimize the KL divergence:

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

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

# Loss functions

Given two distributions $q(z)$ and $p(z)$, the distance between the two distributions can be computed with:

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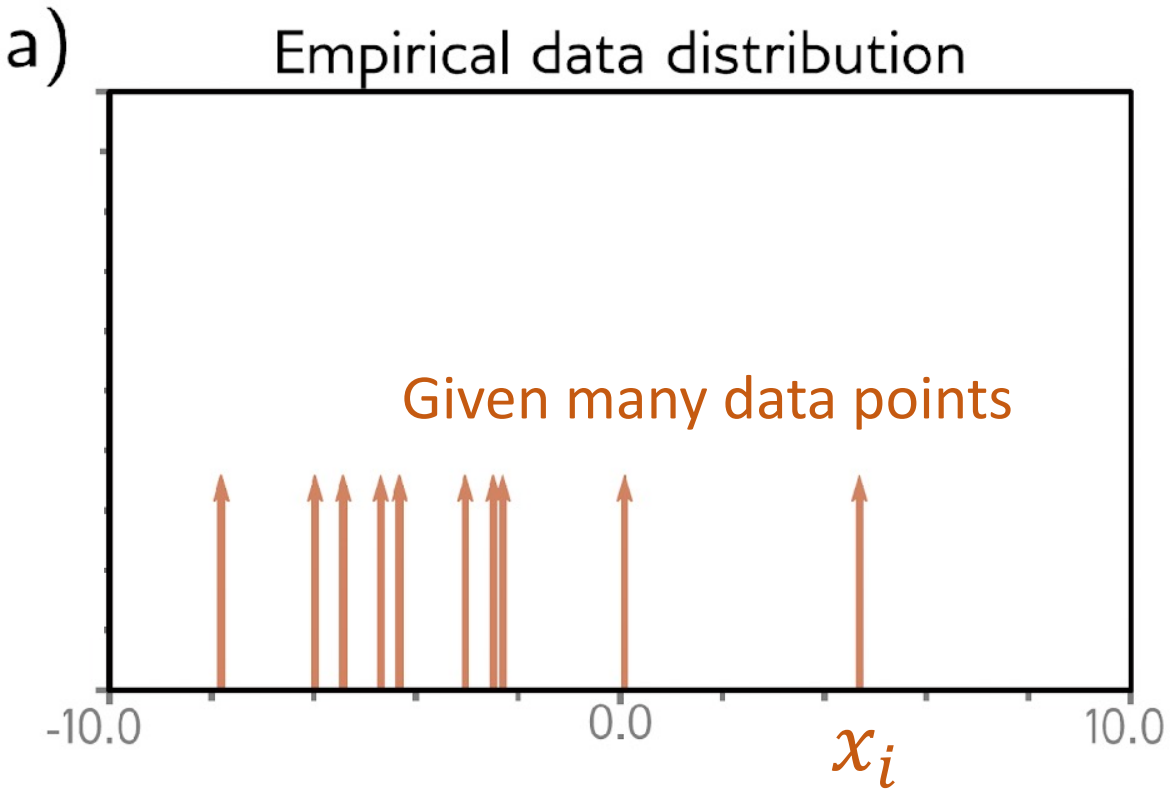
Given an empirical distribution $q(y)$ and a model distribution $Pr(y|\omega)$, we want to minimize the KL divergence:

entropy of q

divergence between q and p

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

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




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

$\delta$: dirac

Source: Understanding Deep Learning, S. Prince, 2023

# Loss functions

Given an empirical distribution $q(y)$ and a model distribution $Pr(y|\omega)$, we want to minimize the KL divergence:

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

cross-entry loss

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

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

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ - \sum_{i=1}^{N} \log[Pr(y_i|\omega)] \right]$$

NLL

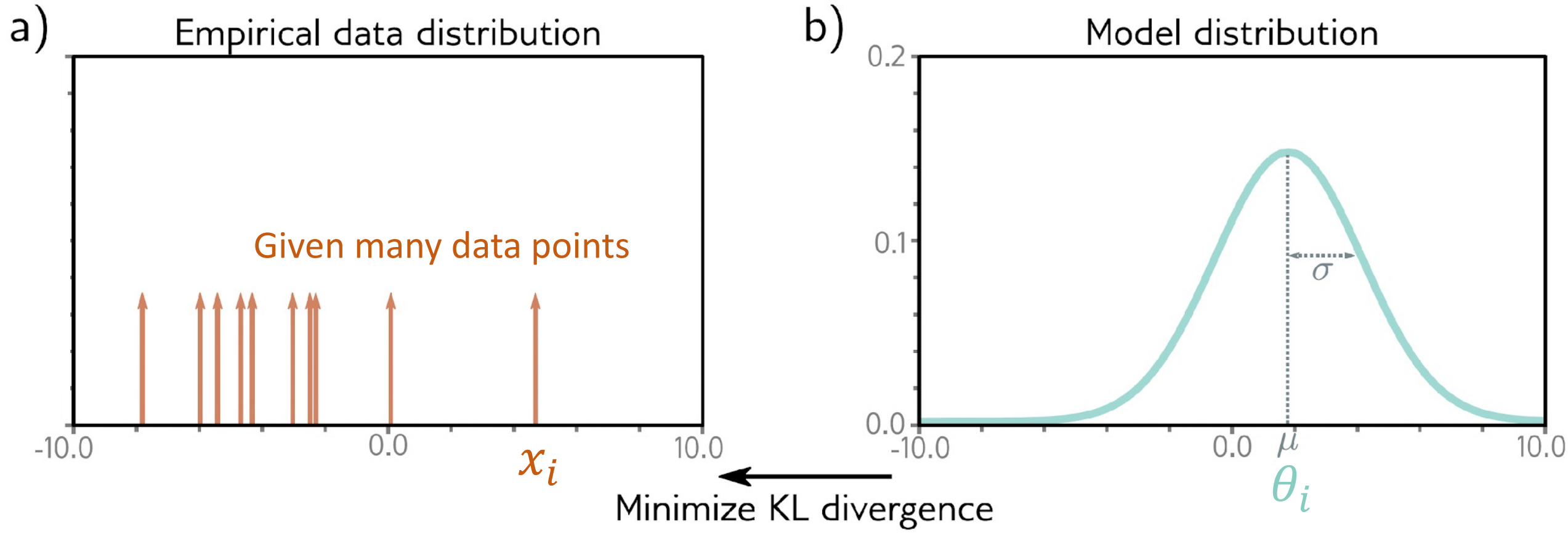



**Figure 5.12** Cross-entropy method. a) Empirical distribution of training samples (arrows denote Dirac delta functions). b) Model distribution (a normal distribution with parameters $\boldsymbol{\theta} = \mu, \sigma^2$). In the cross-entropy approach, we minimize the distance (KL divergence) between these two distributions as a function of the model parameters $\boldsymbol{\theta}$.

Source: Understanding Deep Learning, S. Prince, 2023

# Loss functions

Definition of cross-entropy loss of distribution $p$ relative to distribution $q$ over the set $\mathcal{X}$:

$$H(p, q) = -E_p[\log q]$$

where $E_p[\cdot]$ is the expected value operator with respect to distribution p.

In the continuous case:

$$H(p, q) = -\int_{\mathcal{X}} P(x) \log Q(x)\, dx$$

In the discrete case:

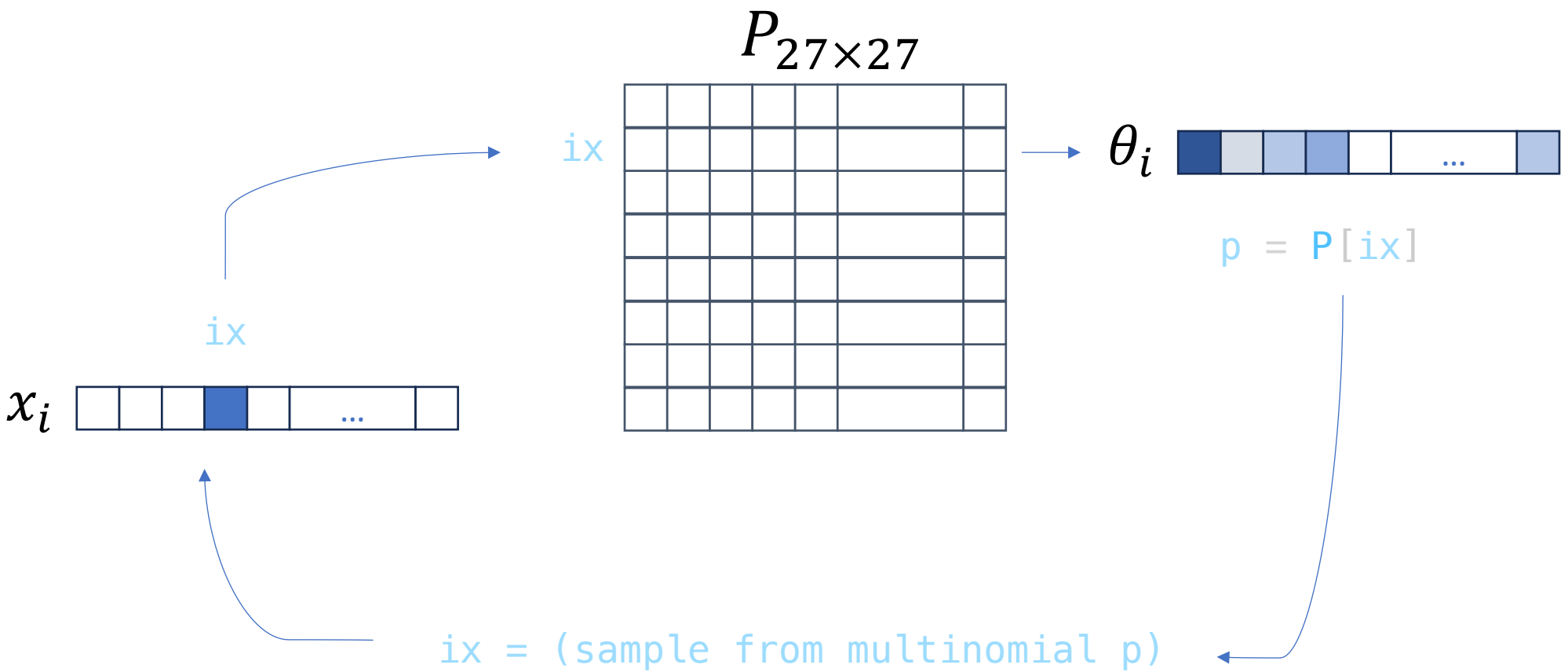
$$H(p, q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x)$$

# TP2: makemore

Goal: Given a bunch of names, generate more “name-like” words.

1. Build a simple bigram model for next-character prediction
2. Build the same bigram model using the NLL loss
3. Implement a better model: [Bengio et al., 2003]

# Step 1: bigram “by hand”



# Step 1: bigram “by hand”

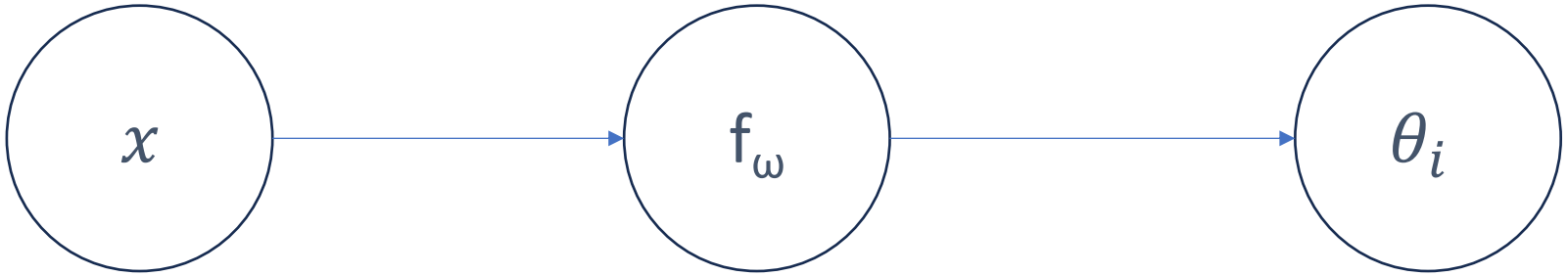
The dot character (.) marks the beginning and end of a word.

When sampling, you need to stop when you hit that special character.

How to initialize a torch matrix of size 27x27 containing floats?

# Step 2: bigram as a learnable matrix

$$f_\omega(x_i) = \theta_i$$




$$x_i = [0,0,0,1,0, \ldots 0]$$

One-hot encoding of letter 'd'

$\omega$ is a matrix $W_{27\times27}$ such that

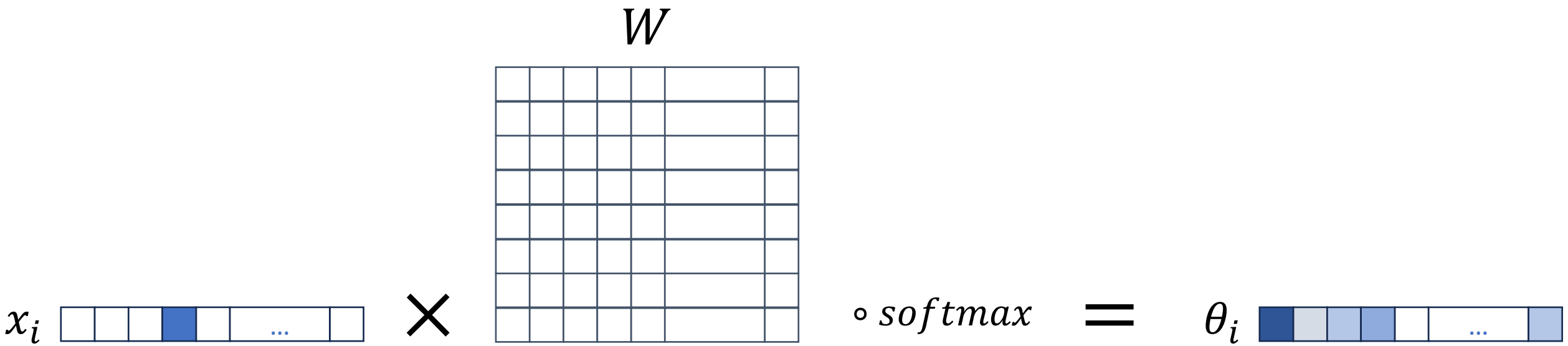
$\theta_i = softmax(x \cdot W)$ is a $N\times27$ vector representing the distribution of the next character for each sample

# Step 2: bigram as a learnable matrix

$x_i$ 

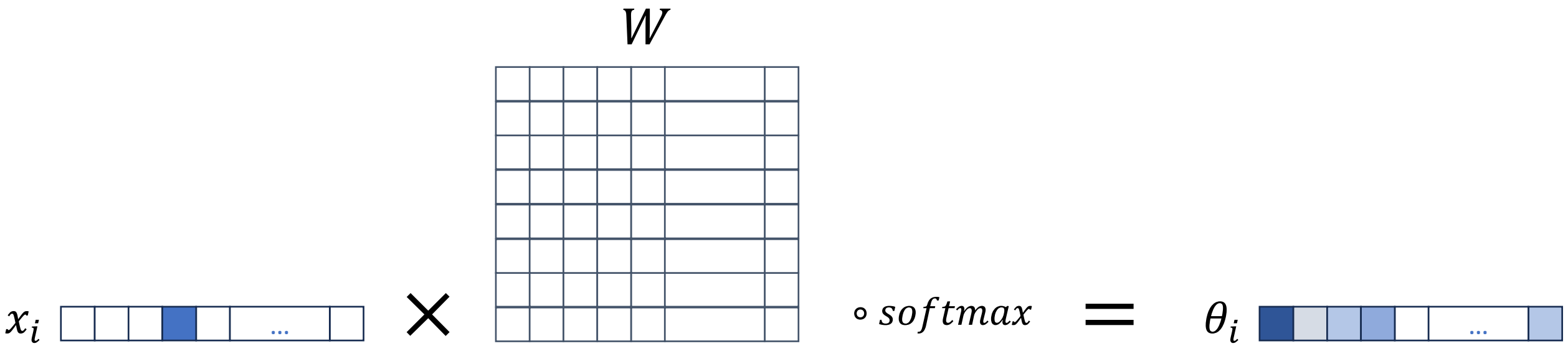

One-hot encoding of letter 'd'

# Step 2: bigram as a learnable matrix




One-hot encoding of letter 'd'

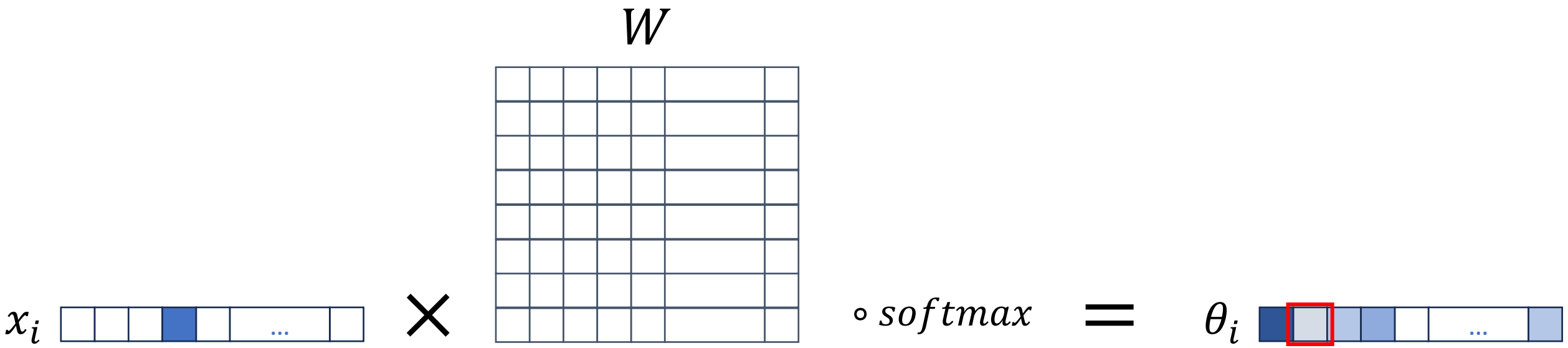
# Step 2: bigram as a learnable matrix




We want to minimize the KL divergence or NLL

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ - \sum_{i=1}^{N} \log[Pr(y_i|\omega)] \right]$$ NLL

# Step 2: bigram as a learnable matrix




We want to minimize the KL divergence or NLL

$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[ -\sum_{i=1}^{N} \log[Pr(y_i|\omega)] \right]$$

NLL

# Step 2: bigram as a learnable matrix

# Step 2: bigram as a learnable matrix

```
#forward pass
xenc = ??? # encode xs with F.one_hot
logits = ??? # multiply by W
counts = ??? # softmax
probs = ???  #
loss = ???   # sum of logs of probs
```

# A few tips...

```
import torch.nn.functional as F
```

$x \cdot W$ is written as `x @ W`

One-hot encoding: `F.one_hot(x, num_classes=...).float()`

For inference `z.multinomial()`

Normalizing a matrix $W_{27\times27}$ by row requires the `keepdim` parameter somewhere...

# A few tips...

```
>>> a = torch.randn((7,7))
>>> a
tensor([[ 1.2555,  0.6821,  0.9131, -0.7238,  0.5636, -2.8689, -0.4744],
        [ 2.1393, -0.8737,  2.4039,  0.0056,  0.6169, -0.2245, -0.2242],
        [ 0.1821, -0.4250, -0.1115, -0.3568, -2.2182,  0.9574,  1.9415],
        [-0.2646,  1.7013, -2.7297,  0.3786, -1.7883,  0.8484, -0.1894],
        [-0.5430, -0.2352,  0.4820, -0.0737,  0.8632,  0.1648,  1.1864],
        [ 1.3596, -0.6411,  2.9097,  0.9422, -0.0167, -0.1453, -0.6059],
        [-0.4946,  0.2705,  0.5348, -1.8176, -1.3861, -1.0276, -1.0050]])
>>> a.sum(axis=1)
tensor([-0.6527,  3.8434, -0.0306, -2.0437,  1.8446,  3.8025, -4.9256])
>>> a.sum(axis=1, keepdim=True)
tensor([[-0.6527],
        [ 3.8434],
        [-0.0306],
        [-2.0437],
        [ 1.8446],
        [ 3.8025],
        [-4.9256]])
```

# Step 3: A Neural Probabilistic Language Model

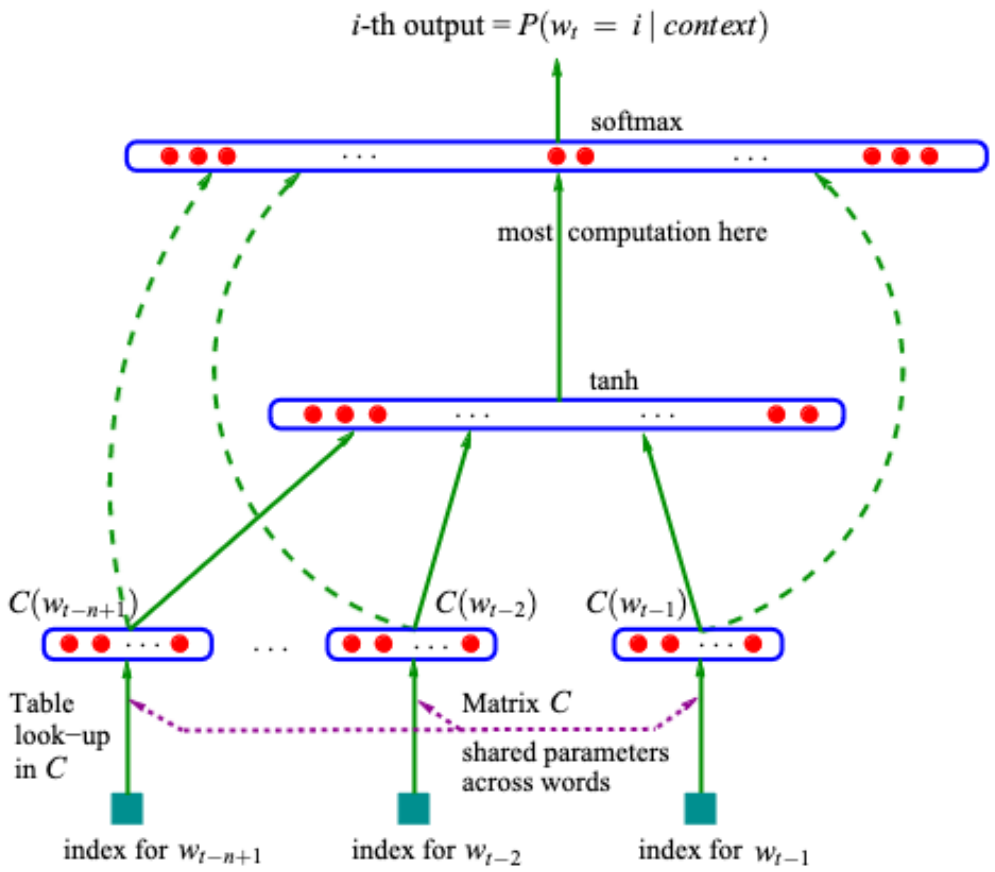


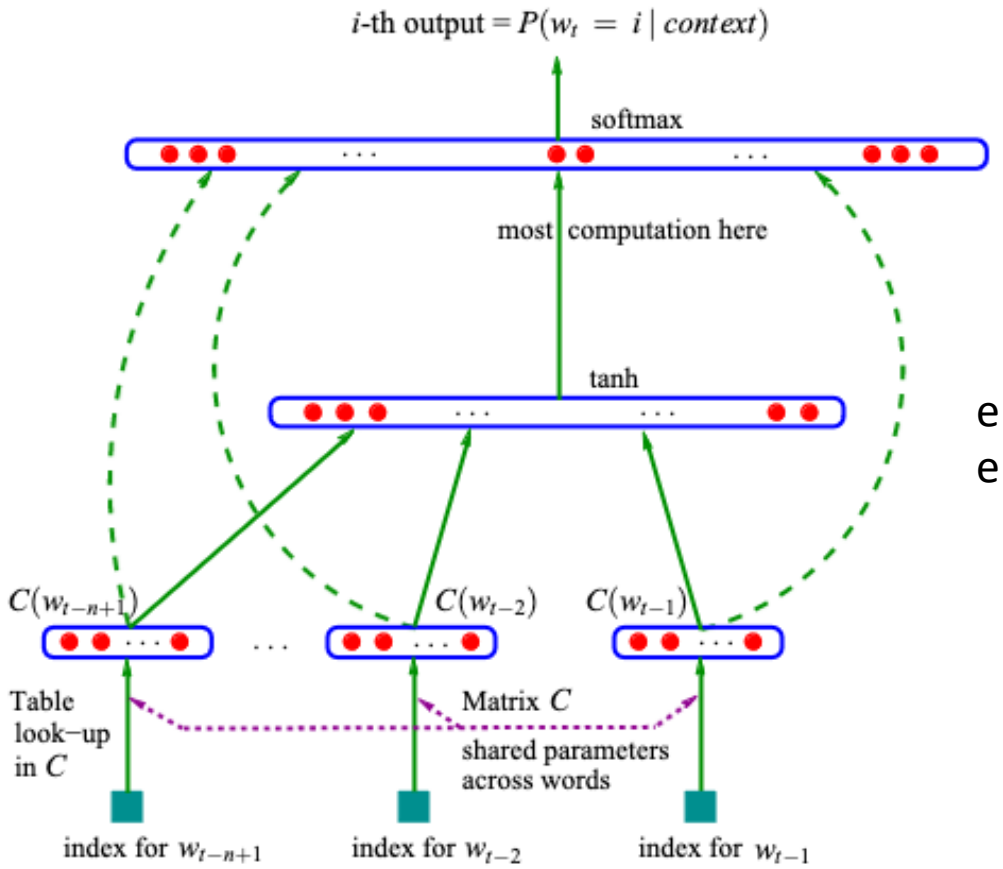

Figure 1: Neural architecture: $f(i, w_{t-1}, \cdots, w_{t-n+1}) = g(i, C(w_{t-1}), \cdots, C(w_{t-n+1}))$ where $g$ is the neural network and $C(i)$ is the $i$-th word feature vector.

A Neural Probabilistic Language Model, Bengio et al, 2003

# Step 3: A Neural Probabilistic Language Model

```
X_train = tensor([
[ 0,  0,  0],
[ 0,  0,  5],
[ 0,  5,  2], ...,
[25,  1, 14],
[ 1, 14, 14],
[14, 14,  9]])
```

$C_{27x10}$= dictionary




$$logits = \tanh(W_2 \cdot h + b_2)$$

$$h = \tanh(W_1 \cdot emb + b_1)$$

emb = C[X_train[ix]]
emb = emb.view(…)

Figure 1: Neural architecture: $f(i, w_{t-1}, \cdots, w_{t-n+1}) = g(i, C(w_{t-1}), \cdots, C(w_{t-n+1}))$ where $g$ is the neural network and $C(i)$ is the $i$-th word feature vector.

A Neural Probabilistic Language Model, Bengio et al, 2003