Deep learning

Unpacking Transformers, LLMs and image generation

Session 2

Syllabus

Session	Lecture	TP
1	Intro to DL Gradient descent and backprop	Intro to micrograd
2	DL fundamentals I • Backprop • Loss functions • Neural Probabilistic Language Model (Bengio 2003)	Bigram model and MLP for next-character prediction
3	DL fundamentals II • Activation function • Regularization • Initialization • Residual networks • Normalization Recurrent Neural Networks	Backprop ninja MLP in pytorch (*) add batchnorm to TP2 (*) MLP for MNIST (Fleuret 3)
4	Attention and Transformers	GPT from scratch (*) Fleuret practical 5 and 6
5	DL for computer vision: convnets, unets	Convnets for Fashion MNIST (*) Fleuret practical 4
6	VAE & Diffusion models	1D diffusion model 2D diffusion model (*) train on GPU **Quiz**

Important notes

Notebooks are scored from 0 to 4.

Always submit a notebook after class. Max score = 1/4 otherwise.

Exercises marked as (*) are required to get to 4. Max score = 2 otherwise.

No class on Feb 21st.

No class on March 27th –> last class on April 3rd. Be there!

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.

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

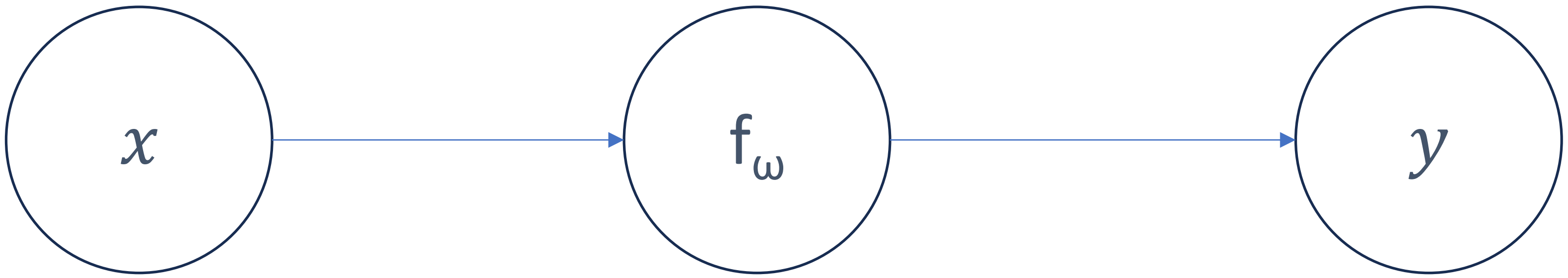
Regularization

Initialization

Residual networks

Batch norm, layer norm

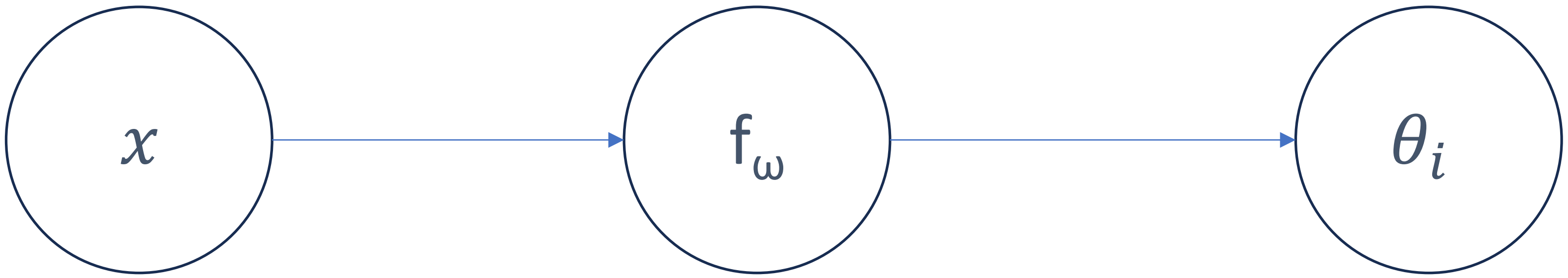
Loss functions



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

ground-truth

Loss functions



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

Parameters of a distribution

Loss functions

$$x \longrightarrow \mathrm{f}_{\omega} \longrightarrow \theta_i$$

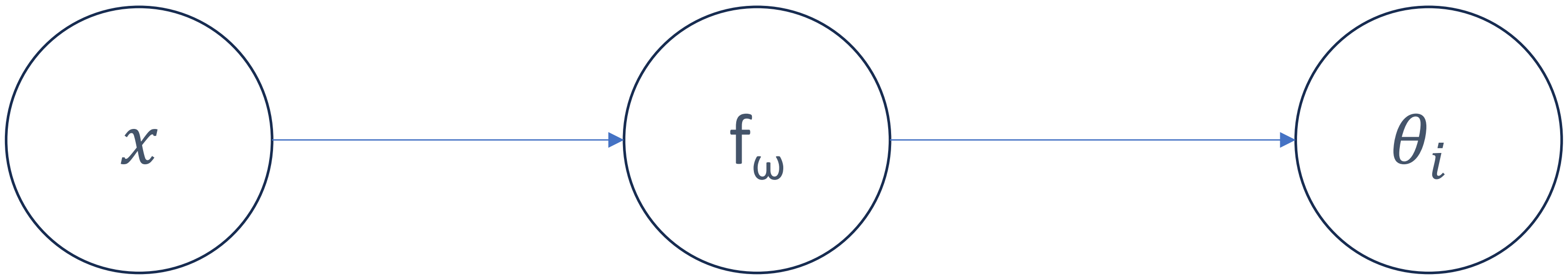
$$f_\omega(x_i) = \theta_i$$

The distribution is chosen based on the domain.

The model computes the optimal θ_i given the data.

Loss functions

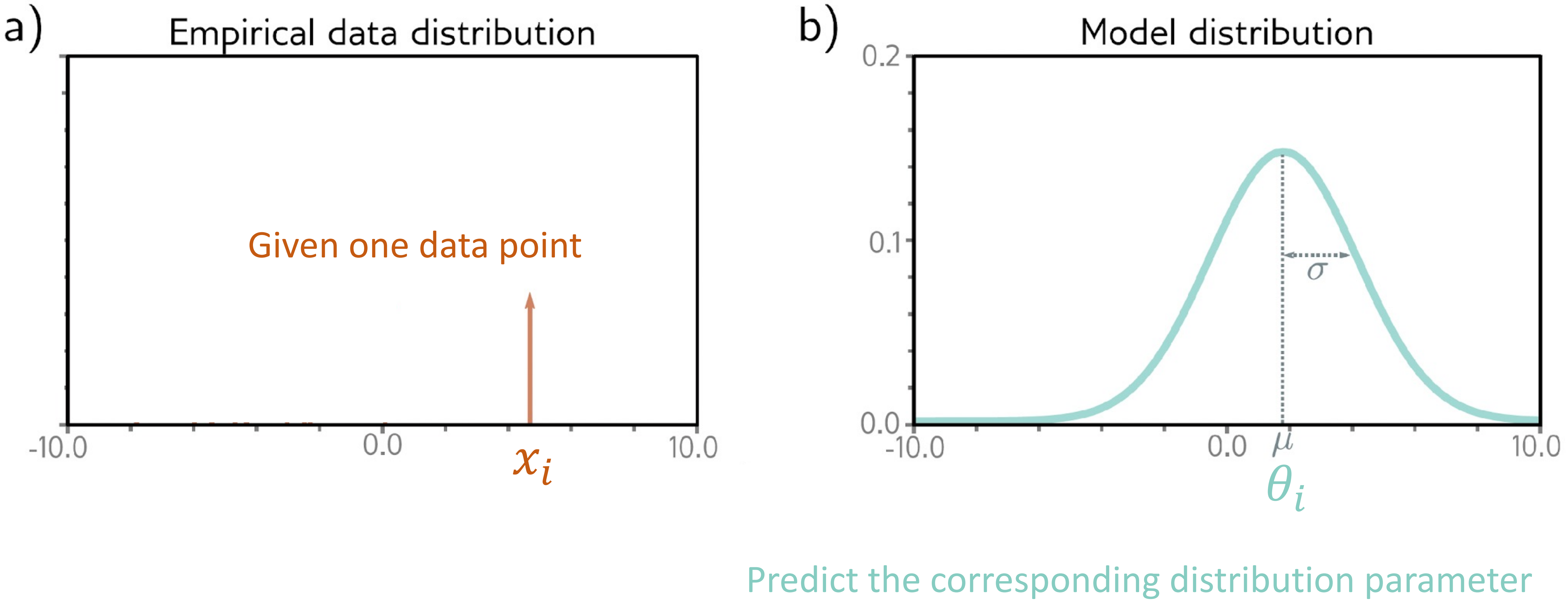
$$f_\omega(x_i) = \theta_i$$

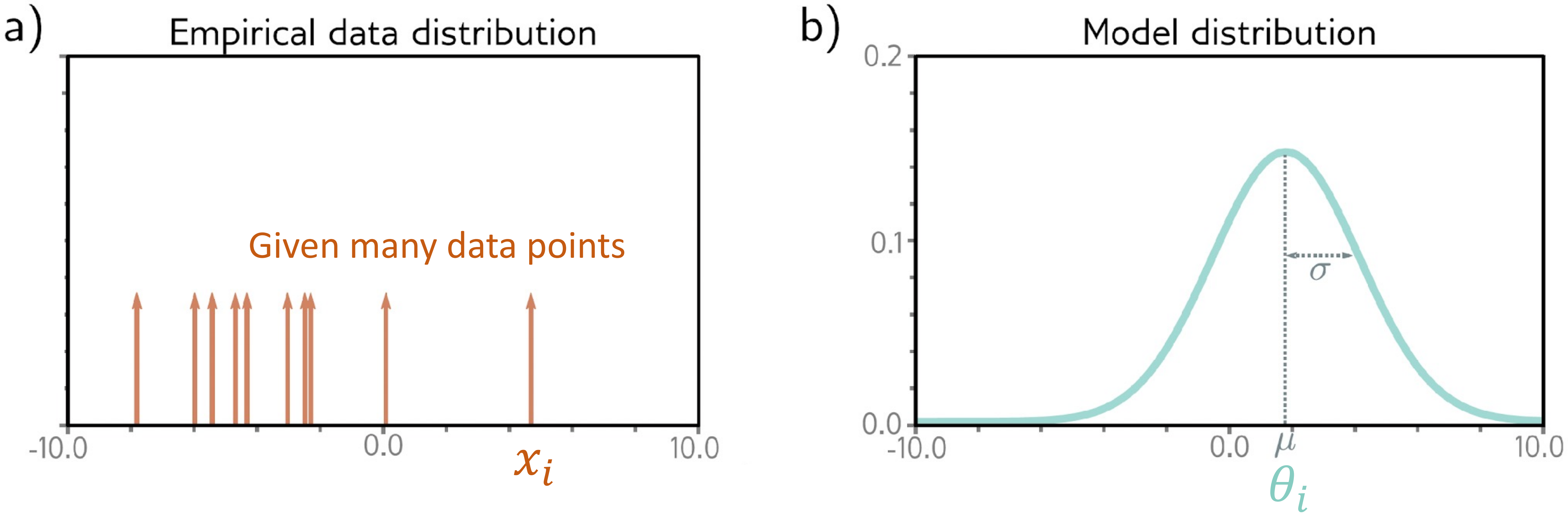


Example: univariate regression

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

θ


a)
Empirical data distribution
Given one data point
-10.0
0.0
10.0
x_i
b)
Model distribution
0.2
0.1
0.0
σ
-10.0
0.0
μ
10.0
θ_i
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

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

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

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

Loss functions

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

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

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

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

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

Negative log likelihood (NLL)

Inference

Given new input data

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

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)

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

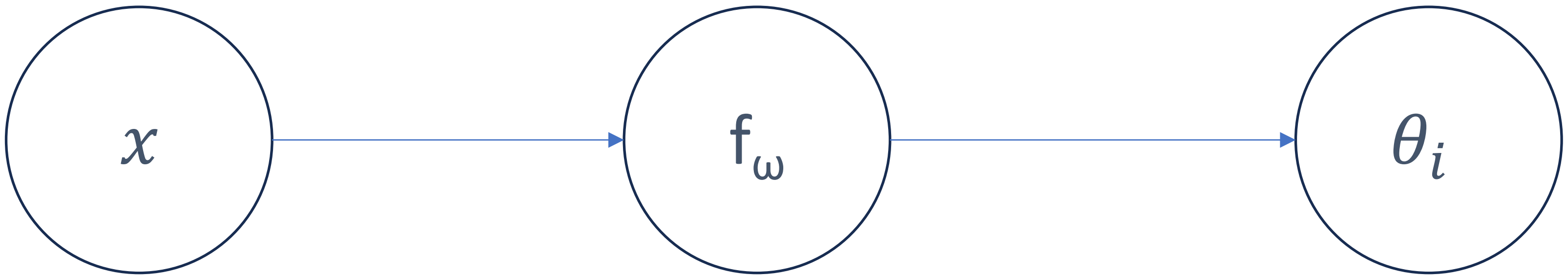
$$\hat{\omega} = \underset{\omega}{\operatorname{argmin}} \left[-\sum_{i=1}^{N} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-f_\omega(x_i))^2}{2\sigma^2}} \right] \right]$$

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

least squares

Loss functions

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



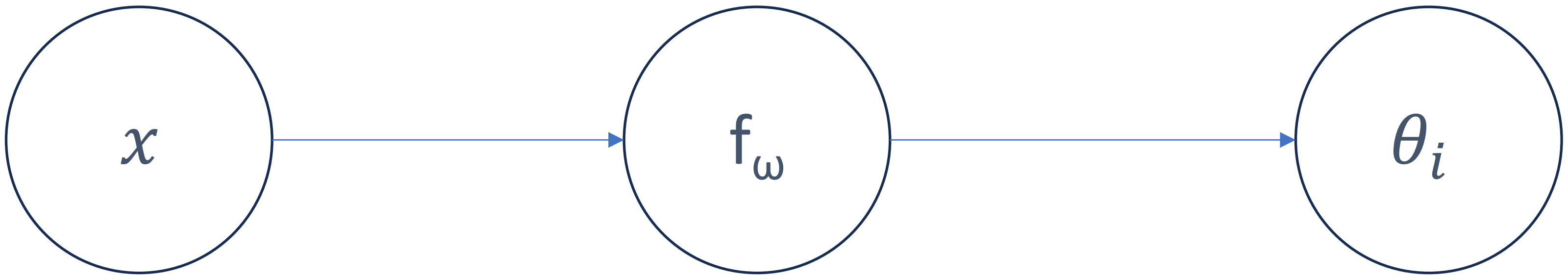
Example: binary classification

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

θ

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

Loss functions

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

$$x \longrightarrow f_\omega \longrightarrow \theta_i$$

Example: multiclass classification

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

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

Loss functions

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

$$x \longrightarrow f_\omega \longrightarrow \theta_i$$

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

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

$$x \longrightarrow f_\omega \longrightarrow \theta_i$$

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:

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

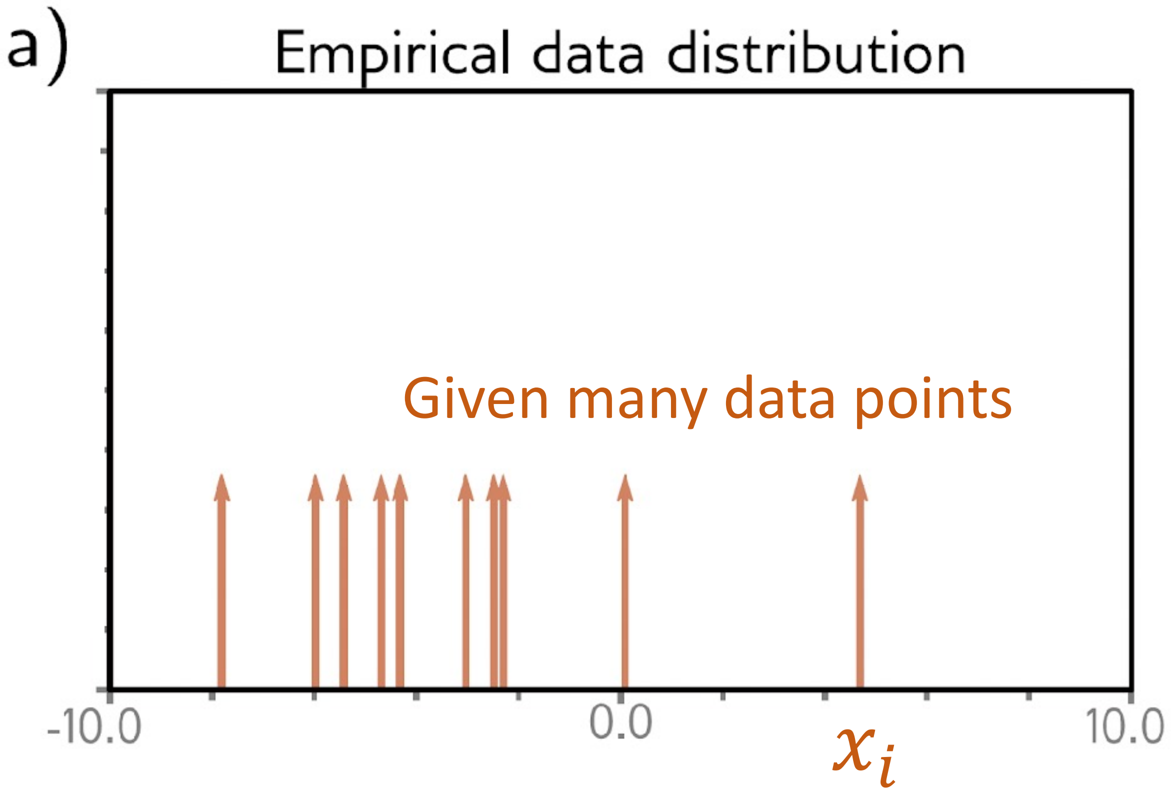
Given an empirical distribution $q(y)$ and a model distribution $Pr(y|\omega)$, we want to minimize the KL divergence:

entropy of q

divergence between q and p

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

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



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

δ: 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

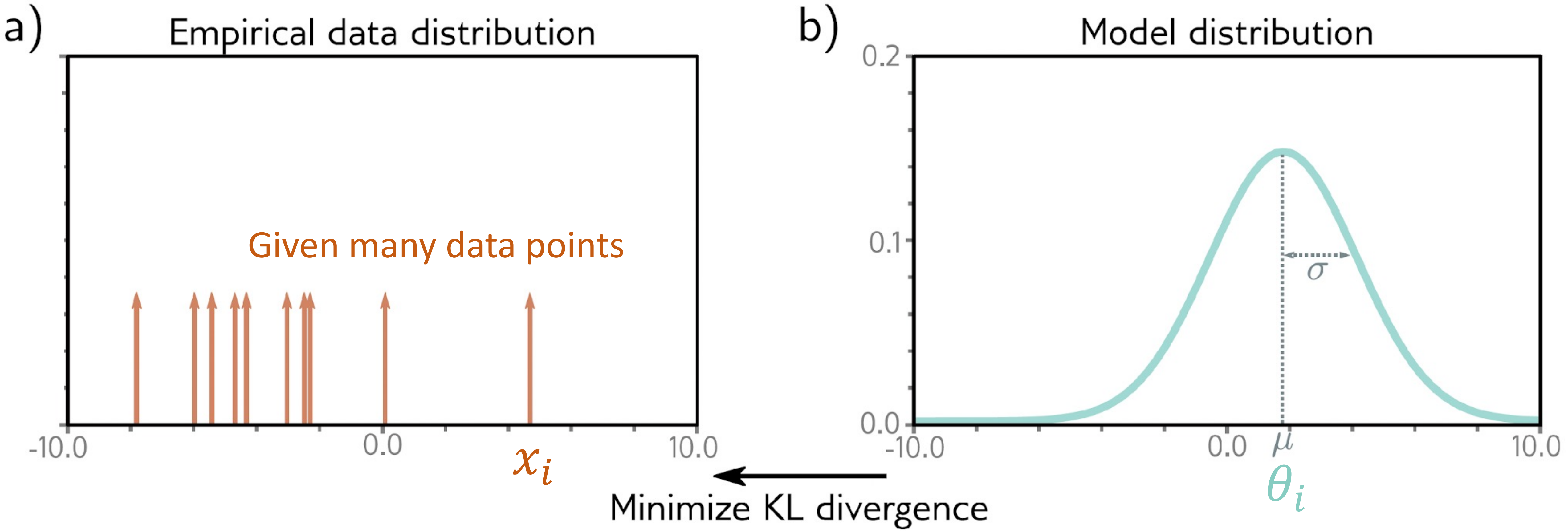


Figure 5.12 Cross-entropy method. a) Empirical distribution of training samples (arrows denote Dirac delta functions). b) Model distribution (a normal distribution with parameters $\boldsymbol{\theta} = \mu, \sigma^2$). In the cross-entropy approach, we minimize the distance (KL divergence) between these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

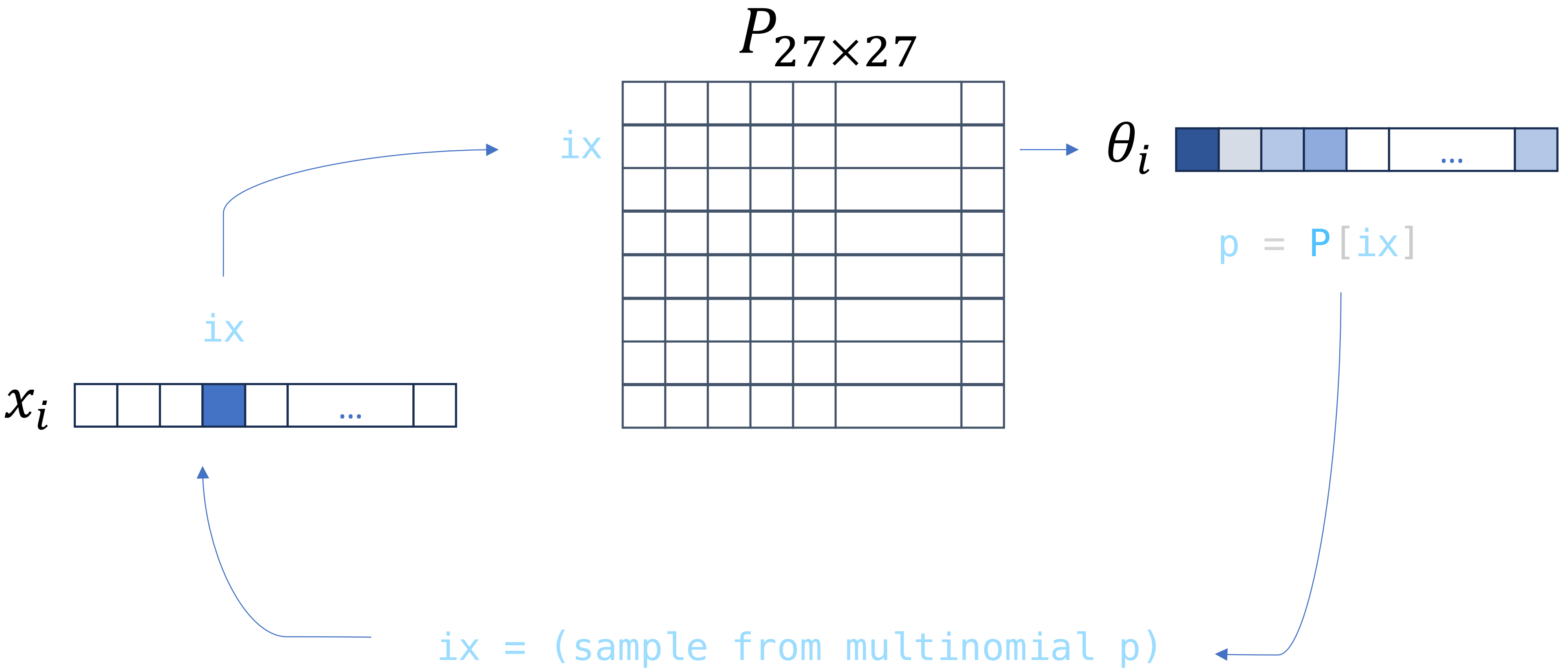
$$H(p,q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x)$$

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”

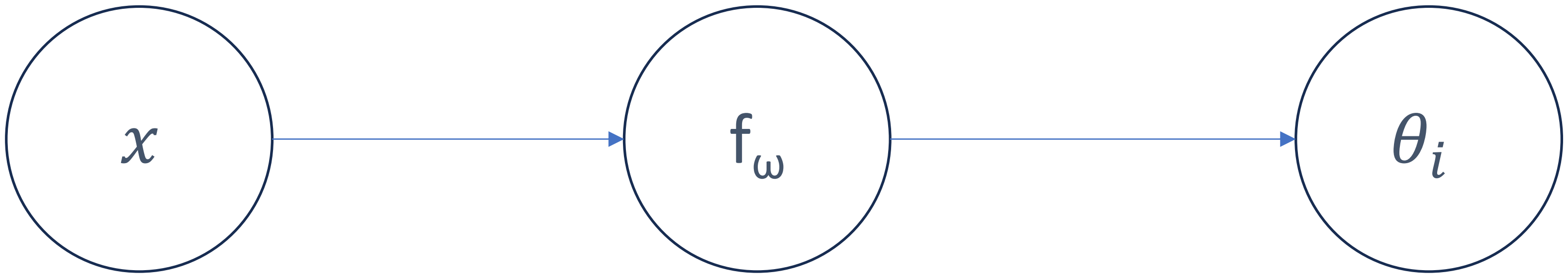
The dot character (.) marks the beginning and end of a word.

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

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



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

One-hot encoding of letter 'd'

ω is a matrix $W_{27\times 27}$ such that

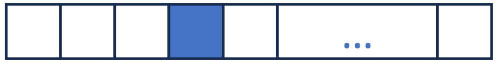
$\theta_i = softmax(x \cdot W)$ is a $N\times 27$ vector

representing the distribution of the next

character for each sample

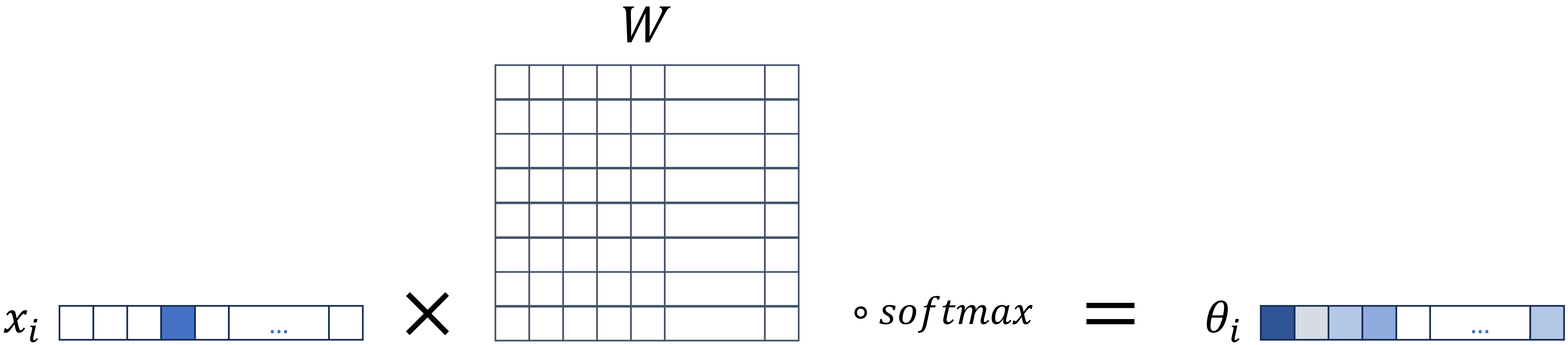
Step 2: bigram as a learnable matrix

x_i



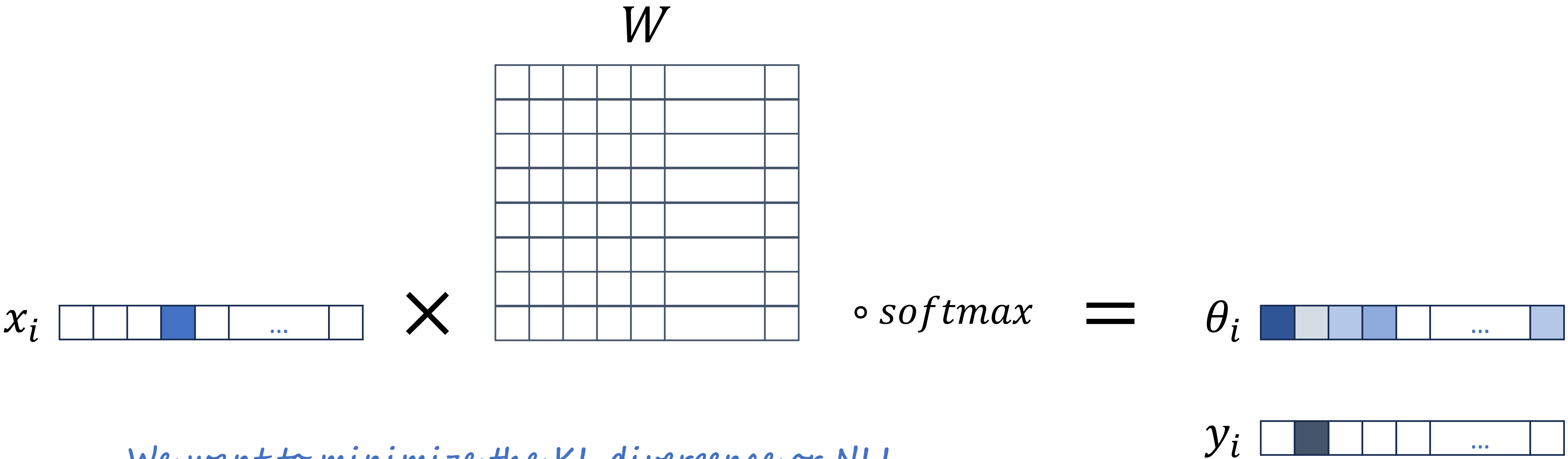
One-hot encoding of letter 'd'

Step 2: bigram as a learnable matrix



One-hot encoding of letter 'd'

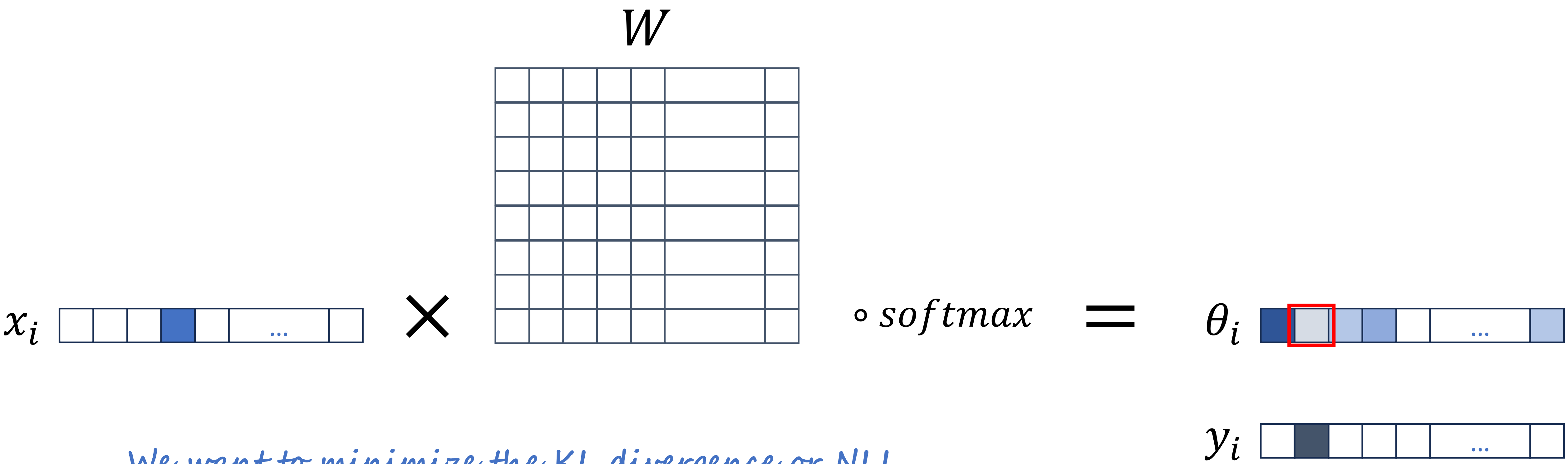
Step 2: bigram as a learnable matrix



We want to minimize the KL divergence or NLL

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

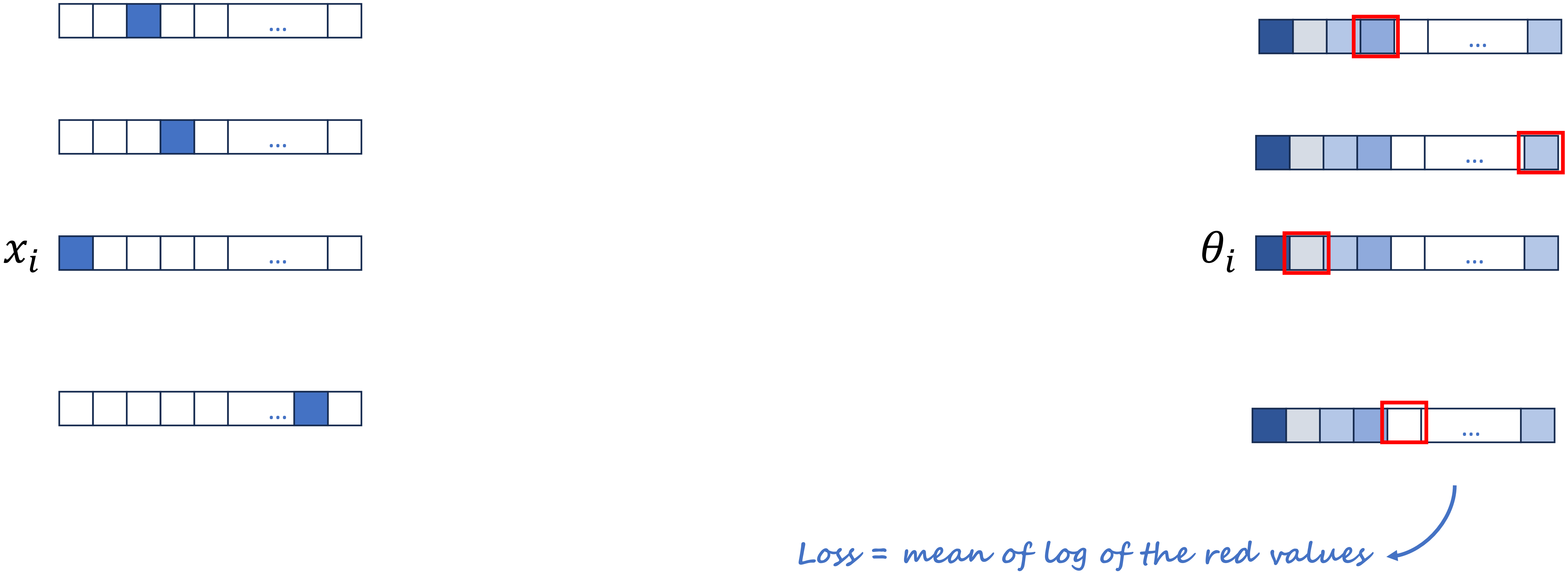
Step 2: bigram as a learnable matrix



We want to minimize the KL divergence or NLL

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

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...

```python
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 $W_{27 \times 27}$ 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

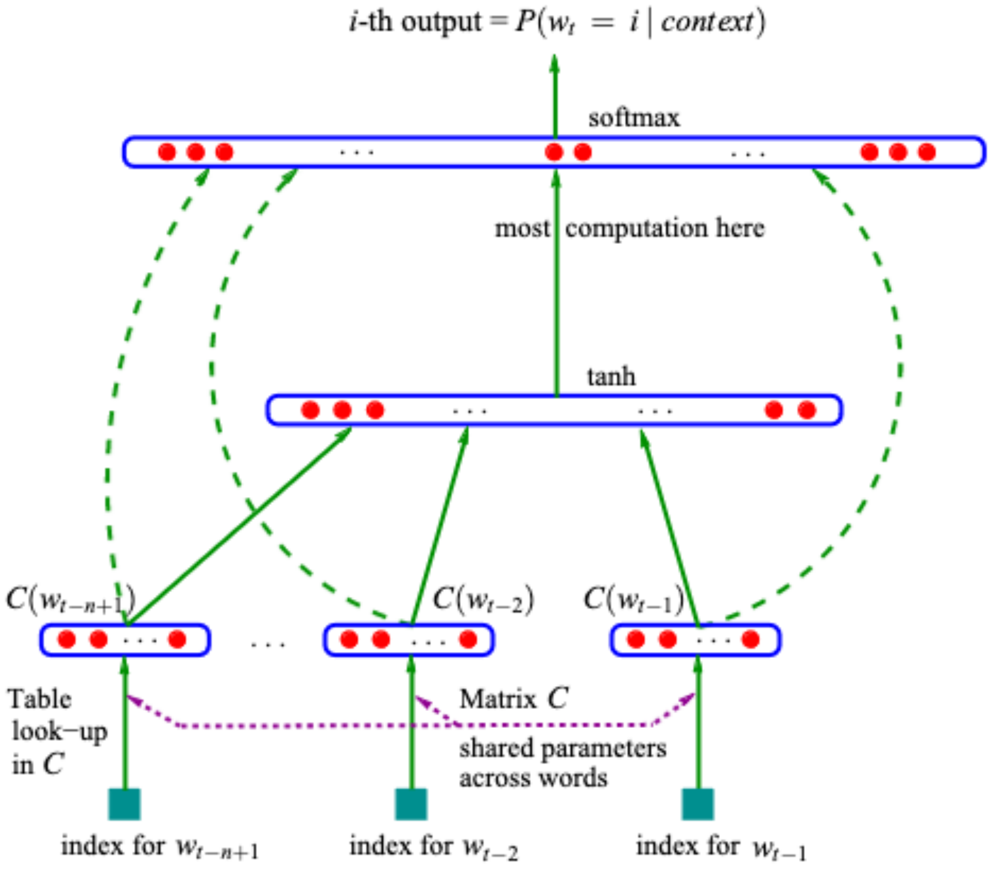


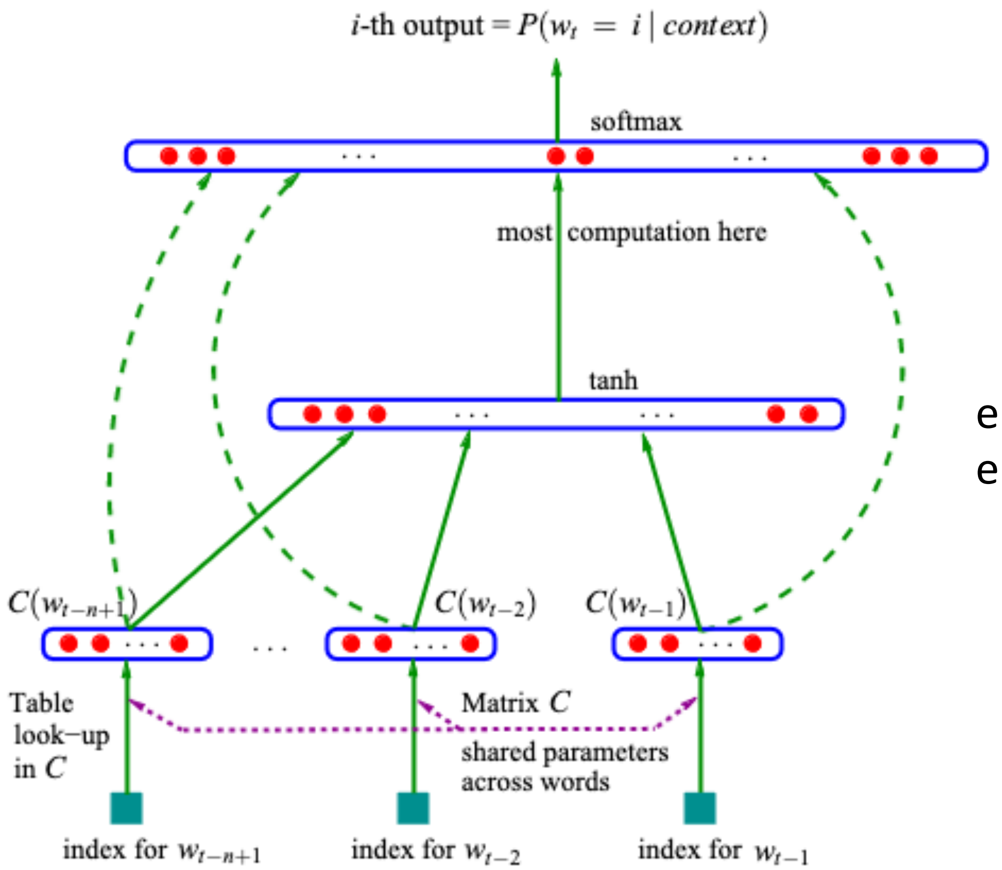
Figure 1: Neural architecture: $f(i, w_{t-1}, \cdots, w_{t-n+1}) = g(i, C(w_{t-1}), \cdots, C(w_{t-n+1}))$ where g is the neural network and $C(i)$ is the i-th word feature vector.

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