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Predictive modeling and unsupervised clustering

Thalita Drumond

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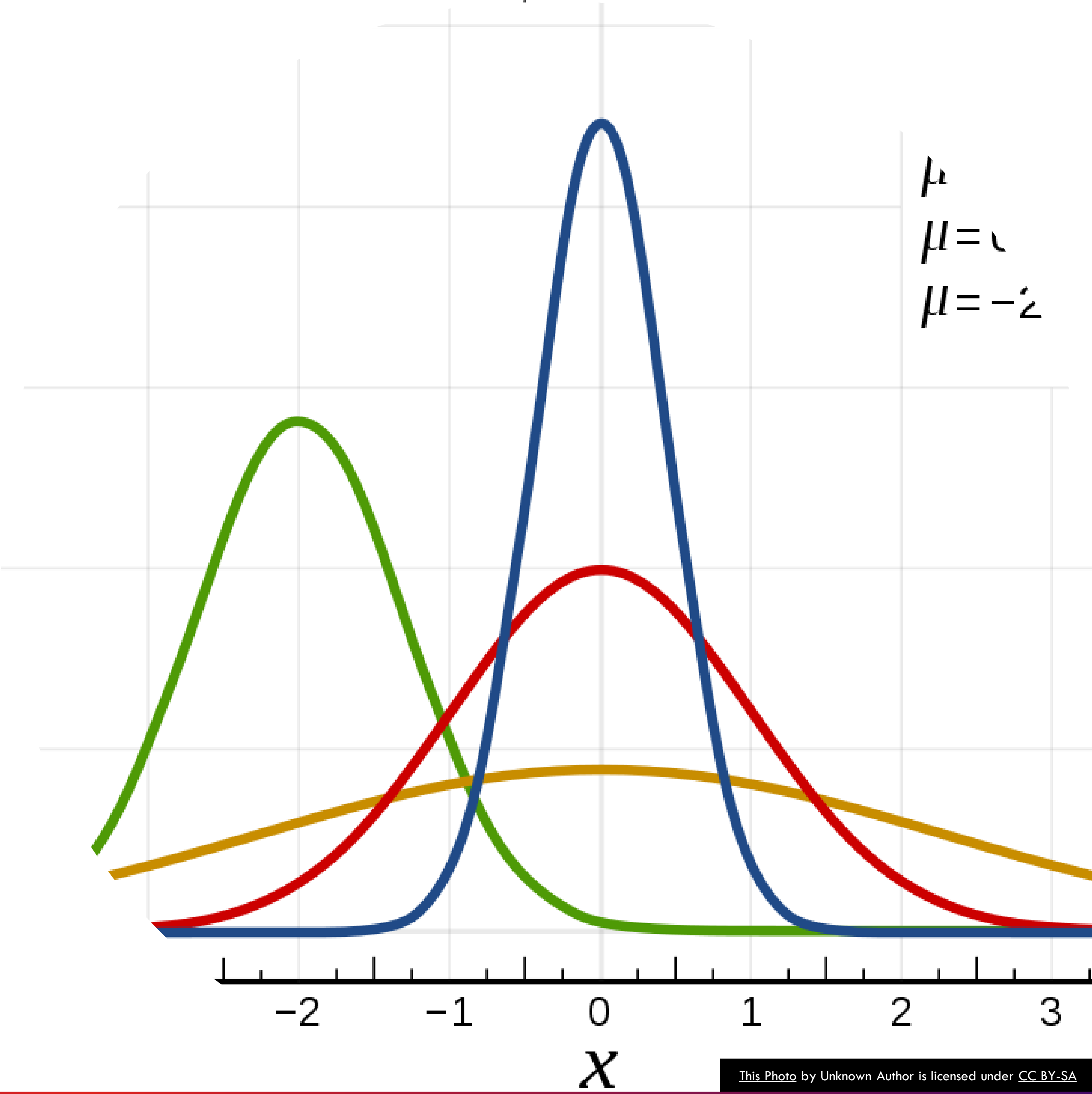
Creating the future together

Extra Exercises

Learning predictive models

Gradient descent for linear regression



GD update with MSE cost function

Ordinary least squares

Minimize the residual sum of squares (RSS):

$$\mathrm{J}(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(\varepsilon^{(i)}\right)^2$$

With $\varepsilon^{(i)}$ being the error between the hypothesis h_θ for input $\boldsymbol{x}^{(i)}$ and the ground truth values $y^{(i)}$:

$$\varepsilon^{(\boldsymbol{i})} := h_\theta\left(\boldsymbol{x}^{(\boldsymbol{i})}\right) - y^{(i)} = \boldsymbol{\theta}^{\boldsymbol{T}}\underbrace{\boldsymbol{x}^{(i)} - y^{(i)}}$$

$\left(\boldsymbol{x}^{(\boldsymbol{i})}, y^{(i)}\right)$ is the i-th sample in the dataset $\mathcal{D}$

Exercise 6

Suppose we will minimize the least-squares cost function using gradient descent:

$$\theta_j[t+1] = \theta_j[t] - \eta\, \Delta\theta_j[t]$$

where η is the learning rate (or step size) and $\Delta\theta_j = \frac{\partial J}{\partial \theta_j}$.

Show that the parameter update is given by $\Delta\theta_j = x_j^{(i)} \varepsilon^{(i)}$

Binary classification with MLE

Binary logistic regression

Binary classification with logistic regression

The hypothesis function is:

$$h_\theta(\boldsymbol{x}) = \sigma\left(\sum_{j=0}^{d} \theta_j x^j\right) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

$$\boldsymbol{\theta}^T : [\theta_1 \cdots \theta_j \ldots \theta_d]$$

Where $\sigma(a)$ is the logistic function:

$$\sigma(a) = \frac{1}{1 + \mathrm{e}^{-a}}$$

$$\boldsymbol{x} : \begin{bmatrix} x^1 \\ \vdots \\ x^j \\ \vdots \\ x^d \end{bmatrix}$$

This hypothesis predicts values of

$$h_\theta(\boldsymbol{x}) \in [0,1]$$

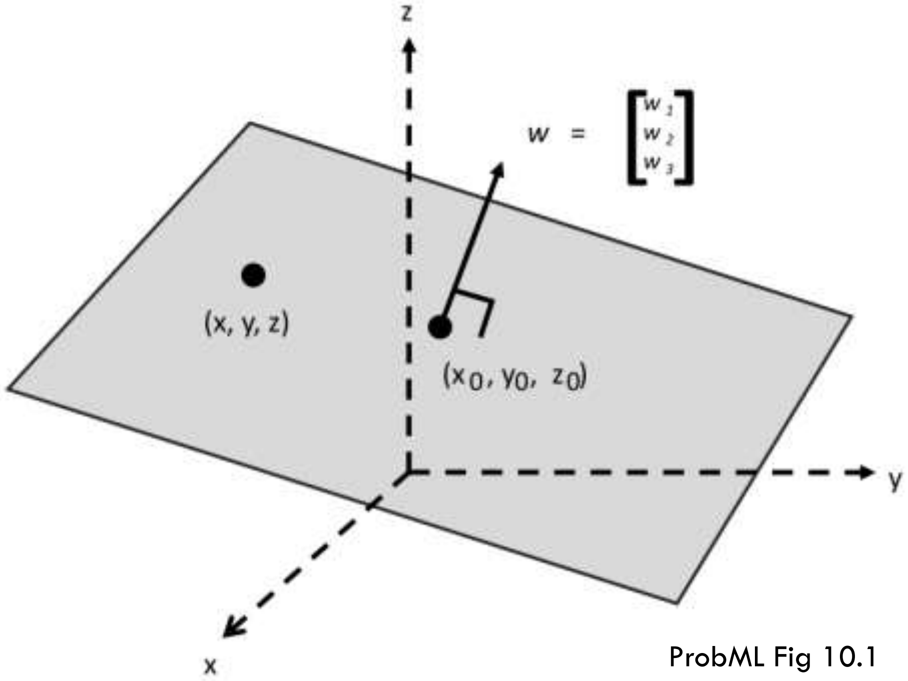
Binary classification with logistic regression

$$p = \text{logistic}(a) = \boldsymbol{\sigma}(a) \triangleq \frac{1}{1 + e^{-a}} = \frac{e^a}{1 + e^a}$$

$$a = \text{logit}(p) = \boldsymbol{\sigma}^{-1}(p) \triangleq \log\left(\frac{p}{1 - p}\right)$$

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \text{Ber}(y|\boldsymbol{\sigma}(\underbrace{w^T x + b}_{a = \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x} + b}))$$

$$p(y = 1|\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{\sigma}(a) = \frac{1}{1 + e^{-a}}$$



ProbML Fig 10.1

Exercise 7

Based on the NLL loss function derived in exercise 4,

$$\mathrm{NLL}(\boldsymbol{\theta}) = -\sum_{i=1}^{N} y_i \log h_\theta(\boldsymbol{x}_i) + (1 - y_i) \log\big(1 - h_\theta(\boldsymbol{x}_i)\big)$$

use the logistic hypothesis

$$p(y = 1 | \boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{\sigma}(a) = \frac{1}{1 + e^{-a}}$$

to write the cost function for logistic regression.

Binary classification with MLE
GD update for logistic regression

Binary classification with MLE
Gradient descent update

NLL cost function:

$$J(\theta) = NLL(\theta) = -\log \mathcal{L}(\theta)$$

$$= -\sum_{i=1}^{N} \boldsymbol{y_i} \log h_\theta(\boldsymbol{x_i}) + (1 - y_i)\log\left(1 - h_\theta(\boldsymbol{x_i})\right)$$

$$\Delta\theta_j \triangleq \frac{\partial}{\partial\theta_j} J(\theta)?$$

Exercise 8

Suppose we will minimize the binary classification NLL cost function using gradient descent:

$$\theta_j[t+1] = \theta_j[t] - \eta\, \Delta\theta_j[t]$$

where η is the learning rate (or step size) and $\Delta\theta_j = \frac{\partial J}{\partial \theta_j}$.

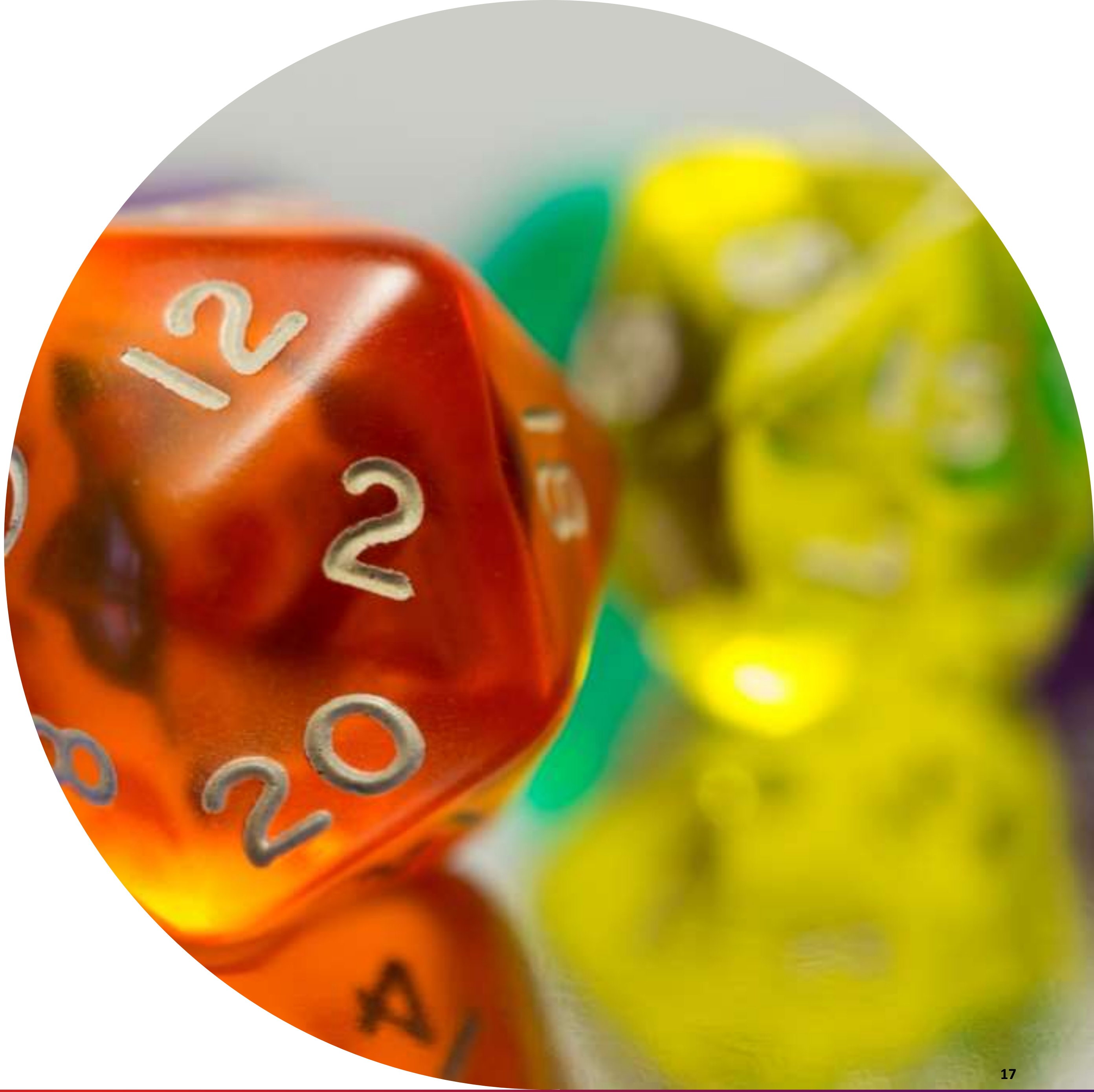
Given the NLL cost function

$$J(\boldsymbol{\theta}) = NLL(\boldsymbol{\theta}) = -\sum_{i=1}^{N} y_i \log h_\theta(\boldsymbol{x}_i) + (1 - y_i) \log\big(1 - h_\theta(\boldsymbol{x}_i)\big)$$

Show that the parameter update is given by $\Delta\theta_j = x_{ij}\varepsilon_i$

Multiclass classification with MLE

Multinomial logistic regression



Multinomial logistic regression

Problem: learn a conditional probability distribution for each class l

$$p(y = l|\boldsymbol{x};\boldsymbol{\theta}) = f_l(\boldsymbol{x};\boldsymbol{\theta})$$

Multinomial logistic regression:

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \mathrm{Cat}(y|\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}))$$

with

$$\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{\mathcal{S}}(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

That is

$$p(y = l|\boldsymbol{x};\boldsymbol{\theta}) = f_l = \mu_l(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

with $\mathbf{W} \subset \mathbb{R}^C \times \mathbb{R}^D$ and $\boldsymbol{\theta} = [\boldsymbol{W};\boldsymbol{b}]$

The **softmax function** is defined as

$$\boldsymbol{\mathcal{S}}: \mathbb{R}^C \to [0,1]^C$$

$$\boldsymbol{\mathcal{S}}(\boldsymbol{a}) \triangleq [\mu_1(\boldsymbol{a}) \quad \cdots \quad \mu_j(\boldsymbol{a}) \quad \cdots \quad \mu_C(\boldsymbol{a})]$$

where

$$\mu_j: \mathbb{R}^C \to [0,1]$$

$$\mu_j(\boldsymbol{a}) = \frac{\exp(-a_j)}{\sum_{l=1}^{C} \exp(-a_l)}$$

$\boldsymbol{a}$ values are called **logits**

Exercise 9

Based on the NLL loss function derived in exercise 5,

$$NLL(\theta) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{l=1}^{C} y_{il}\log f_{il}$$

use the softmax hypothesis

$$\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{\mathcal{S}}(\mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

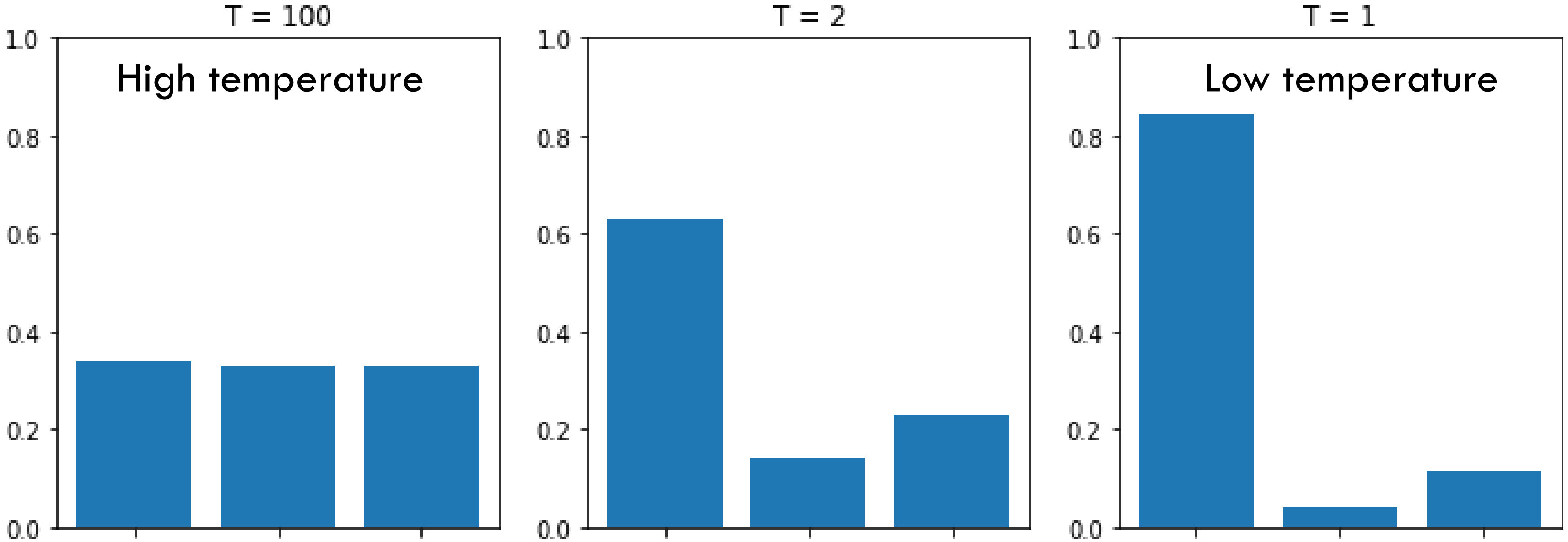
to write the cost function for multinomial logistic regression.

Softmax function with temperature

High temperature → uniform distribution
Low temperature → true max selection

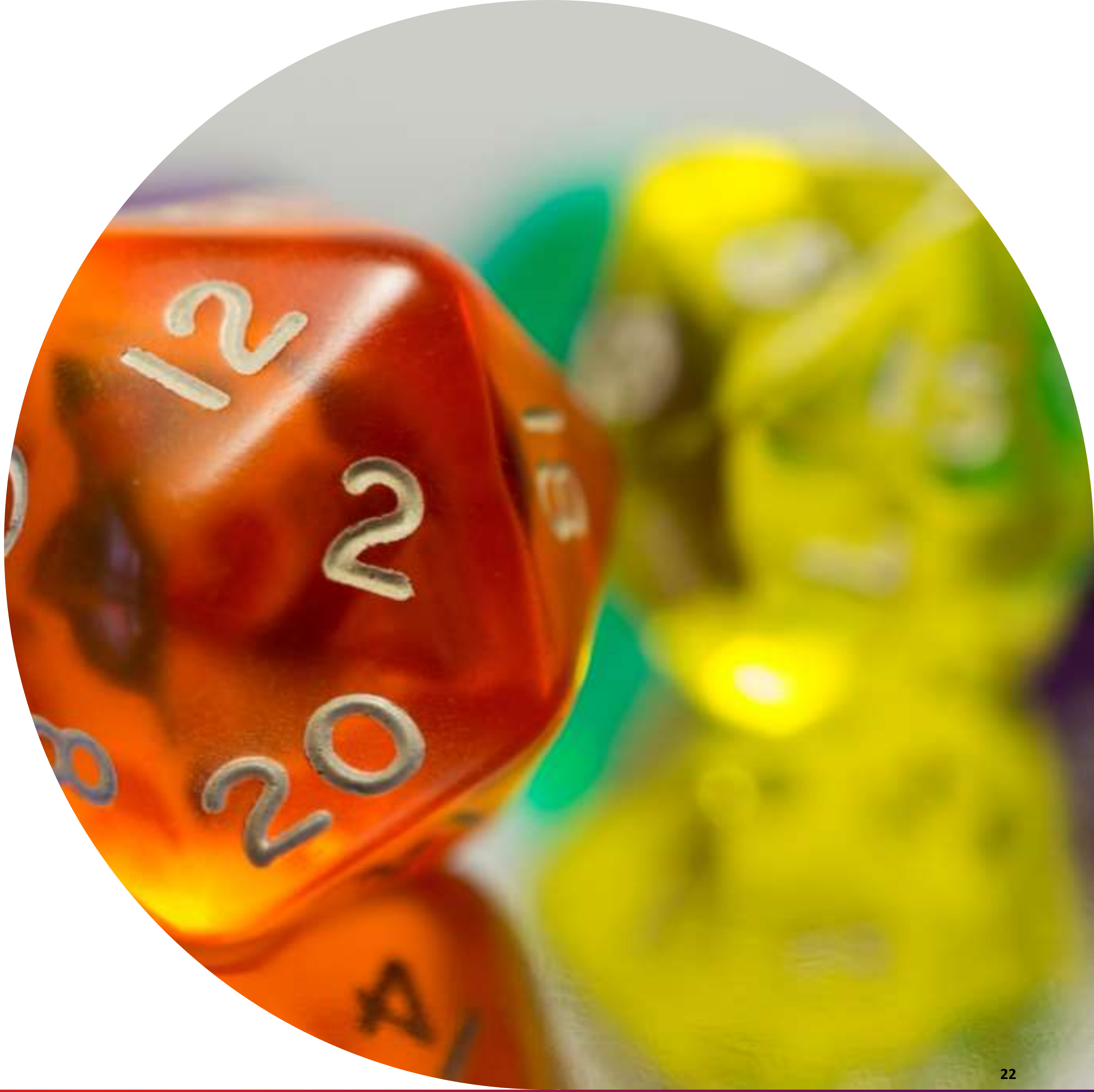
As $T \to 0$

$$\mathcal{S}(\boldsymbol{a}/T)_c = \begin{cases} 1.0 & \text{if } c = \operatorname{argmax}_{c'} a_{c'} \\ 0.0 & \text{otherwise} \end{cases}$$



ProbML Section 2.5, Figure 2.12

Multiclass classification with MLE
GD update



Multiclass classification with MLE
GD update

NLL cost function:

$$J(\theta) = \frac{1}{N} NLL(\theta) = -\frac{1}{N} \sum_{n=1}^{N} \sum_{c=1}^{C} y_{nc} \log \mu_{nc}$$

with $\mu_{nc} = \mu_{nc}(\boldsymbol{a}) = \frac{\exp(-a_{nc})}{\sum_{\mathrm{j}=1}^{C} \exp(-a_{nj})}$ and $\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x}$ (assume the $\boldsymbol{b}$ term to be included in W)

Gradient descent update:

$$\Delta\theta_j \triangleq \frac{\partial}{\partial \theta_j} J(\theta)?$$

Exercise 10

We are going to show that the parameter update $\Delta\theta_j = \frac{\partial J}{\partial \theta_j}$ is AGAIN given by $\Delta\theta_j = x_{ij}\varepsilon_i$.

We will assume the weight matrix $\boldsymbol{D} \times \boldsymbol{C}$ is flattened into a $\boldsymbol{CD}$ vector.

1. First, use the chain rule to decompose the derivative as follows

$$\nabla_{\boldsymbol{w}_j} NLL_n = \sum_c \frac{\partial NLL_n}{\partial \mu_{nc}} \frac{\partial \mu_{nc}}{\partial a_{nj}} \frac{\partial a_{nj}}{\partial \boldsymbol{w}_j}$$

   where $\boldsymbol{w}_j$ denotes the vector of weights associated with class j

2. Then compute the partial derivatives.
   a) (optional) It can be derived that for any sample, $\frac{\partial \mu_c}{\partial a_j} = \mu_c\left(\delta_{cj} = \mu_j\right)$, where $\delta_{cj} = \mathbb{I}(c = j\ )$.
   b) Show that $\frac{\partial NLL_n}{\partial \mu_{nc}} = -\frac{y_{nc}}{\mu_{nc}}$
   c) Show that $\frac{\partial a_{nj}}{\partial \boldsymbol{w}_j} = \boldsymbol{x}_n$

3. Use these three partial derivatives to show that

$$\nabla_{\boldsymbol{w}_j} NLL_n = \left(\mu_{nj} - y_{nj}\right)\boldsymbol{x}_n$$

Empirical risk minimization

Empirical risk minimization cost function

Average **loss** of the predictive model on the training set

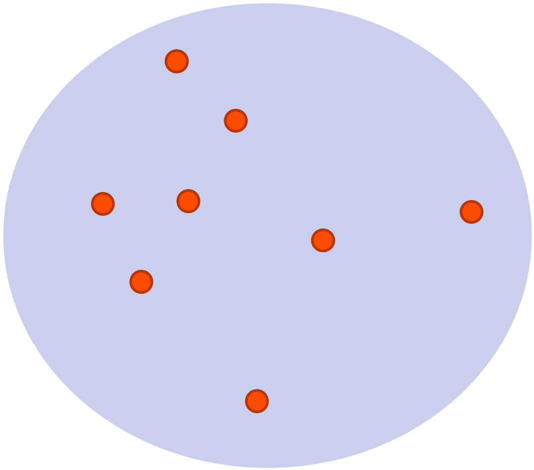
$$\mathcal{L}(\theta) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \ell(\boldsymbol{y}_n, \boldsymbol{\theta}; \boldsymbol{x}_n)$$

Empirical distribution of the dataset $\mathcal{D}$ with samples $\boldsymbol{y}_n \sim p(\boldsymbol{Y})$:

$$p_{\mathcal{D}}(\boldsymbol{y}_n) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \delta(\boldsymbol{y} - \boldsymbol{y}_n)$$

i. e., δ-functions centered at each sample $\boldsymbol{y}_n$:

Data distribution $p(X, Y)$



Dataset samples $(\boldsymbol{x}_n, \boldsymbol{y}_n) \in \mathcal{D}$

Samples are drawn from data distribution $\boldsymbol{x}_n, \boldsymbol{y}_n \sim p(\mathcal{X}, \mathcal{Y})$

Empirical risk minimization

Example using least-squares error

Cost = Mean squared error

$$\mathcal{L}(\theta) \stackrel{\text{def}}{=} \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{y}_n - f(\boldsymbol{x}_n;\theta))^2$$

Here the loss is the squared error:

$$\ell(\boldsymbol{y}_n, \boldsymbol{\theta}; \boldsymbol{x}_n) = (\boldsymbol{y}_n - f(\boldsymbol{x}_n;\theta))^2$$

Empirical risk minimization
Example using misclassification rate

Cost = Misclassification rate

$$\mathcal{L}(\theta) \stackrel{\text{def}}{=} \frac{1}{N}\sum_{n=1}^{N} \underbrace{\mathbb{I}(\boldsymbol{y}_n \neq f(\boldsymbol{x}_n; \theta))}$$

Counts the number of misclassified samples

$$\mathbb{I}(e) = \begin{cases} 1 & \text{if } e \text{ is true} \\ 0 & \text{if } e \text{ is false} \end{cases}$$

Here the loss is the Indicator function

$$\ell(\boldsymbol{y}_n, \boldsymbol{\theta}; \boldsymbol{x}_n) = \mathbb{I}(\boldsymbol{y}_n \neq f(\boldsymbol{x}_n; \theta))$$

Exercise 11

MLE is equivalent to empirical risk minimization (under a particular loss)

Looking back to the negative log likelihood cost function derived in exercise 1, compare it to the empirical risk cost function and identify the loss $\ell(\boldsymbol{y}_n, \boldsymbol{\theta}; \boldsymbol{x}_n)$ that makes both cost functions equivalent.

Summary

	Hypothesis $p(y\|\boldsymbol{x};\boldsymbol{\theta}) = p(y\|h_\theta(\boldsymbol{x}))$	Error derivative $\varepsilon_i = h_\theta(\boldsymbol{x_i}) - y_i$ $\frac{\partial}{\partial\theta_j}\varepsilon_i = \frac{\partial}{\partial\theta_j}h_\theta(\boldsymbol{x_i})$	Loss	Parameter update for a single sample $\boldsymbol{x_i}$ $\boldsymbol{\nabla}_{\theta_j}\mathrm{NLL}(\boldsymbol{\theta})$
Linear regression	$\mathcal{N}(y\|\boldsymbol{\theta}^T\boldsymbol{x}, \sigma^2)$	x_{ij}	MSE	$\Delta\theta_j = \varepsilon_i x_{ij}$
Logistic regression	$\mathrm{Ber}\big(\mathrm{y}\|\sigma(\boldsymbol{\theta}^T\boldsymbol{x})\big)$ $\sigma(z) = \frac{1}{1+\mathrm{e}^{-z}}$	$\sigma'(x_{ij})x_{ij}$	Cross-entropy	$\Delta\theta_j = \varepsilon_i x_{ij}$
Multinomial logistic regression	$\mathrm{Cat}\big(y\|\boldsymbol{\mathcal{S}}(\boldsymbol{\theta}^T\boldsymbol{x})\big)$ $p(y=k\|x;\theta) = [\boldsymbol{\mathcal{S}}(\boldsymbol{\theta}^T\boldsymbol{x})]_k$ $[\boldsymbol{\mathcal{S}}(\boldsymbol{a})]_j = \mu_j(\boldsymbol{a}) = \frac{\exp(-\mathrm{a}_j)}{\sum_{\mathrm{k}=1}^{C}\exp(-a_k)}$	$\mu_l\big(\delta_{lj} - \mu_j\big)x_{ij}$ $= \begin{cases} 0 & if\ j = l \\ -\mu_l\mu_j x_{ij} & if\ j \neq l \end{cases}$	Cross-entropy	$\Delta\boldsymbol{\theta}_j = \varepsilon_i\boldsymbol{x_i}$