Machine Learning

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- *ERM*
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- *Ridge Regression (L_2 regularization)*
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1.1 Basic Knowledge

Example 1.1 Linear Regression

Settings.

- Dataset: $D = \{(x_i, y_i)\}_{i=1}^n$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. Here, y_i denotes the regression target, while x_i represents the input features used to predict y_i.
- Linear Model: $f(x) = W^\top x + b$, with weight $W \in \mathbb{R}^d$ and bias $b \in \mathbb{R}$.

Note *This definition is equivalent to an inner product: $\hat{y} = W^\top x + b$.*

Definition 1.1 (Learnable / Trainable Parameters)

Learnable parameters are those that can be updated during the training process.

Quiz. How to determine whether a parameter is learnable? Quiz: How to determine W and b?

Ans: **ERM** (Empirical Risk Minimization)

- Loss function. Squared Loss (SE) is commonly used during optimization. The training objective can be written as:

$$\underset{W,b}{\operatorname{argmin}} \frac{1}{n} \sum_{i \in [n]} (y_i - (W^\top x_i + b))^2 \tag{1.1}$$

The blue factor $1/n$ can be omitted in theoretical analysis, but is often kept in practice to stabilize the loss function during implementation.

Quiz: How to optimize the parameters?

Ans: **Gradient Descent** (as a traditional ML method). In the case of linear regression:

$$\frac{\partial \mathcal{L}}{\partial b} = -2 \sum_{i \in [n]} (y_i - W^\top x_i - b) \tag{1.2}$$

$$\frac{\partial \mathcal{L}}{\partial W} = -2 \sum_{i \in [n]} (y_i - W^\top x_i - b) x_i \tag{1.3}$$

Note *In the field of machine learning, the gradient of a scalar with respect to a vector is itself a vector* ***(not a covector)****. This means:*

$$\frac{\partial \mathcal{L}}{\partial W} = \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial W_1} \\ \frac{\partial \mathcal{L}}{\partial W_2} \\ \vdots \\ \frac{\partial \mathcal{L}}{\partial W_d} \end{pmatrix} = \left(\frac{\partial \mathcal{L}}{\partial W_1}, \frac{\partial \mathcal{L}}{\partial W_2}, \cdots, \frac{\partial \mathcal{L}}{\partial W_d} \right)^\top \tag{1.4}$$

Note *Here are some commonly used derivative formulas:*

$$\frac{\partial x^\top x}{\partial x} = 2x \tag{1.5}$$

$$\frac{\partial a^\top x}{\partial x} = a, \quad \frac{\partial A x}{\partial x} = A^\top \tag{1.6}$$

$$\frac{\partial x^\top A x}{\partial x} = (A + A^\top) x \tag{1.7}$$

Remark Both sides of an equation must have the same dimension. This principle can be used as a consistency check.

We optimize the parameters by subtracting a scalar multiple of the gradient from the parameters, considering the physical meaning of the gradient: the direction of the steepest **increase**.

Definition 1.2 (Hyperparameter)

A parameter that is fixed during optimization and specified before the training process. ♣

That is:

$$W' = W - \alpha \frac{\partial \mathcal{L}}{\partial W}, \quad b' = b - \alpha \frac{\partial \mathcal{L}}{\partial b} \tag{1.8}$$

Optimization will stop when the norm of the parameter update becomes smaller than a given hyperparameter.

1.2 Closed-Form of Linear Regression

Proposition 1.1

*Linear Regression has **Closed-Form** solution.* ♡

Settings.

- Metrix $X_0 := (x_1^\top, \cdots, x_n^\top)^\top$;
- Metrix $X := (X_0, \mathbb{1}) \in \mathbb{R}^{n\times(d+1)}$;
- $y = (y_1, \cdots, y_n)^\top \in \mathbb{R}^n$;
- $\hat{w} = (w, b)^\top \in \mathbb{R}^{d+1}$.

Then the loss function of $\hat{w}$ can be writtern as:

$$\mathcal{L}(\hat{w}) = (y - X\hat{w})^\top (y - X\hat{w}) = \|y - X\hat{w}\|_2^2 \tag{1.9}$$

Here, $\|\cdot\|_p$ denotes the *p-norm* of a vector.

Note *Vectors can sometimes be treated as scalars, since linearity ensures that the validity of a proposition can be extended to any finite dimension.*

Notice that the optimization stops when $\partial\mathcal{L}(\hat{w})/\partial\hat{w} = 0$. Under this condition, the parameters can be solved from the above constraint by following steps:

$$\frac{\partial \mathcal{L}(\hat{w})}{\partial \hat{w}} = -2X^\top (y - X\hat{w}) \tag{1.10}$$

Note *Both dimensional analysis and calculation using Leibniz's rule lead to the same result as the formula above:*

$$\begin{aligned} \mathcal{L}(\hat{w}) &= y^\top y - 2y^\top X\hat{w} + \hat{w}^\top X^\top X\hat{w} \\ \partial_{\hat{w}}\mathcal{L}(\hat{w}) &= -2X^\top y + 2X^\top X\hat{w} \\ &= -2X^\top (y - X\hat{w}) \end{aligned}$$

Remark More matix formulas are available in Matrix Cookbook.

Thus, the target of the optimization satisfied:

$$X^\top y = X^\top X\hat{w} \tag{1.11}$$

That is:

$$\hat{w} = (X^\top X)^{-1} X^\top y \tag{1.12}$$

when $X^\top X$ invertible (non-singular / full-rank).

Example 1.2 When does $X^\top X$ not invertible?

Solution $X \in \mathbb{R}^{n\times(d+1)}$:

- $d + 1 > n$. *Brief Proof:* $\operatorname{rank}(X^\top X) = \operatorname{rank}(X) \le \min(n, d+1) = n < d + 1$.
- *X has repeated columns. Proof is trivial.*

When $X^\top X$ isn't invertible:

1. If $\operatorname{rank}(X^\top X, X^\top y) > \operatorname{rank}(X^\top X)$, $\hat{w}$ has no solution;
2. $\hat{w}$ has infinity solution o.w.

Situation 1 is **Impossible** because both $X^\top X$ and $X^\top y$ can be represented in the column space of $X^\top$. Therefore, the optimization problem must have a solution, which may be either unique or infinite.

As an infinite set of solutions makes it difficult to determine which estimate of $\hat{w}$ to choose, we apply L_2 **regularization** to linear regression, which is commonly referred to as **Ridge Regression**. That is:

$$\mathcal{L}_{L_2} := \mathcal{L}(\hat{w}) + \boxed{\lambda\|\hat{w}\|_2^2} \tag{1.13}$$

Noticed that $\|\hat{w}\|_2^2 = \sum_{i=1}^{d+1} \hat{w}_i^2$, L_2 regularization prevents any single dimension from being assigned an excessively large weight, , and encourages the model to make use of more dimensions during training.

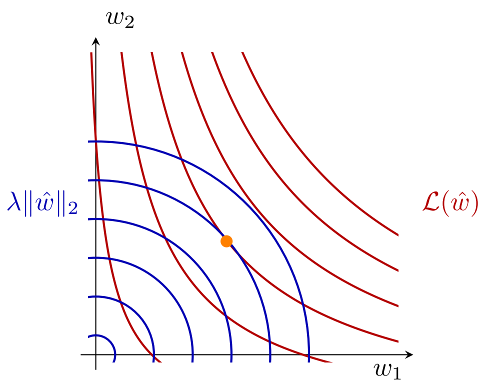

Figure 1.1: Illustration of L_2 regularization. The contours represent level sets of the regularized loss $\mathcal{L}(\hat{w}) + \lambda\|\hat{w}\|_2^2$, which take the form of concentric ellipses (circle in the plot).

During ridge regression, we minimize the $\mathcal{L}_{L_2}$:

$$\operatorname*{argmin}_{\hat{w}} (y - X\hat{w})^\top (y - X\hat{w}) + \lambda \hat{W}^\top \hat{W} \tag{1.14}$$

The optimization stops when:

$$\frac{\partial \mathcal{L}_{L_2}}{\partial \hat{w}} = -2X^\top y + 2X^\top X\hat{w} + 2\lambda I\hat{w} = 0 \tag{1.15}$$

$$\Rightarrow (X^\top X + \lambda \mathbb{I})\hat{w} = X^\top w \tag{1.16}$$

Proposition 1.2

$X^\top X + \lambda\mathbb{I}$ always invertible. ♡

Proof Since $X^\top X$ is a real symmetric matrix, we have the eigen-decomposition $X^\top X = U\Lambda U^\top$, where $\Lambda = \operatorname{diag}(\lambda_1, \cdots, \lambda_{d+1})$. Moreover, as $X^\top X \succeq 0$ is positive semi-definite, it follows that $\forall i \in [d+1]$, $\lambda_i \geq 0$. Note that:

$$\lambda\mathbb{I} = \lambda U U^\top \tag{1.17}$$

since U is an orthogonal matrix. Hence:

$$X^\top X + \lambda\mathbb{I} = U(\Lambda + \lambda I)U^\top \tag{1.18}$$

For all $i \in [d+1]$, we have:

$$\lambda_i + \lambda > \lambda_i \geq 0 \tag{1.19}$$

Thus, $X^\top X + \lambda I$ is a full-rank matrix.

Remark Numerical issues may still occur even if $X^\top X$ is full rank (e.g., when eigenvalues λ_k are close to zero). The L_2 regularization factor λ mitigates this issue by shifting the eigenvalues upward, thereby improving numerical stability during training.

Another regularization method often used is L_1 regularization, where the loss function is defined as:

$$\mathcal{L}_{L_1} := \mathcal{L}(\hat{w}) + \boxed{\lambda\|\hat{w}\|_1} \tag{1.20}$$

L_1 regularization can induce sparsity in $\hat{w}$, which works in contrast to L_2 regularization. Specifically, L_1 regularization encourages the model to rely on only a small subset of input features, effectively performing **feature selection**.

Linear regression with L_1 regularization is called **Lasso Regression** (Least Absolute Shrinkage and Selection Operator).

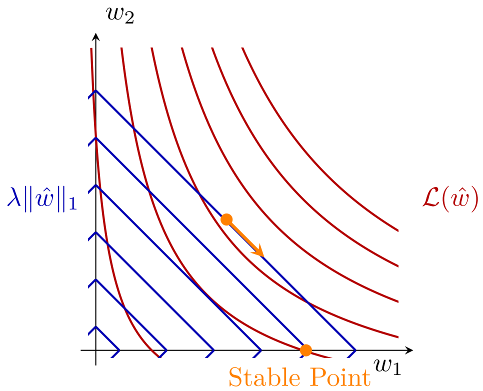

Figure 1.2: Illustration of L_1 regularization. The contours represent level sets of the regularized loss $\mathcal{L}(\hat{w}) + \lambda\|\hat{w}\|_1$, which take the form of nested diamonds (squares rotated by 45° in the plot).

1.3 Geomeric View of LR

Ideally, we would like to solve $X\hat{w} = y$. If y lies on the hypersurface

$$\mathcal{M}(X) := \mathrm{Span}(X) = \{Xw : w \in \mathbb{R}^d\} \subset \mathbb{R}^n \tag{1.21}$$

then the equation admits an exact solution. In most cases, however, $y \notin \mathcal{M}(X)$, so no exact solution exists. Nevertheless, we can always find an estimator $\hat{w}$ such that $\mathcal{P}_{\mathcal{M}(X)}y = X\hat{w}$, where $\mathcal{P}_{\mathcal{M}(X)}$ denotes the orthogonal projection onto the hypersurface $\mathcal{M}(X)$.

Proposition 1.3

$$\hat{y} = X\hat{w} \quad \Rightarrow \quad \hat{w} \textit{ is solution to LR.} \tag{1.22}$$

♡

Proof

$$\begin{aligned} y - \hat{y} \perp \mathcal{M}(X) \quad &\Rightarrow \quad y - X\hat{w} \perp \mathcal{M}(X) \\ &\Rightarrow \quad X^\top(y - X\hat{w}) = 0 \quad \Rightarrow \quad \hat{w} = (X^\top X)^{-1}X^\top y \end{aligned}$$

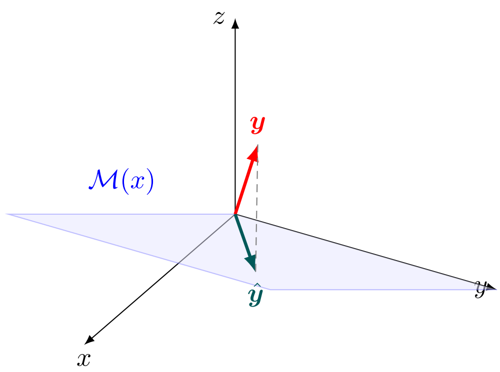

Figure 1.3: Orthogonal projection interpretation of linear regression. The predicted vector $X\hat{w}$ is obtained as the projection of y onto the hypersurface $\mathcal{M}(X) = \{Xw : w \in \mathbb{R}^d\}$, which is a linear subspace in the classical case.

Chapter 2 Logistic Regression

Introduction

- *Binary Classification Problem*
- *Cross Entropy*
- *Sigmoid Regression*
- *Maximum a posteriori*

Example 2.1 **Binary Classification Problem**

Settings.

- Dataset: $D = \{(x_i, y_i)\}_{i=1}^n$, where $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$. Here, y_i denotes the classification target, while x_i represents the input features used to predict y_i.
- Model in Logistic Regression: In logistic regression, we start with a linear model $f(x) = w^\top x + b$. Unlike in ordinary regression, where the target variable lies in $\mathbb{R}$, here the target space collapses to $\{0, 1\}$. Thus, we need a function that maps real-valued outputs into this discrete set. Moreover, in many applications it is desirable to obtain not only a hard classification decision (0 or 1), but also a *soft* prediction: the probability of each class. Such a probabilistic interpretation provides both the likelihood estimate and the corresponding classification outcome.

Can we directly use a linear model to fit $p(y = 1 \mid x = x_i)$, as we did in the previous chapter? The answer is *no*. This is because there is a mismatch between the range of a linear model output (which lies in $\mathbb{R}$) and the valid domain of probabilities, $[0, 1]$.

To resolve this issue, we introduce a transformation function called the **sigmoid** function. The sigmoid maps any real-valued input into the interval $[0, 1]$, making it suitable for modeling probabilities. It is defined as:

Definition 2.1 (Sigmoid Function)

$$\sigma(z) = \frac{1}{1 + e^{-z}} \tag{2.1}$$

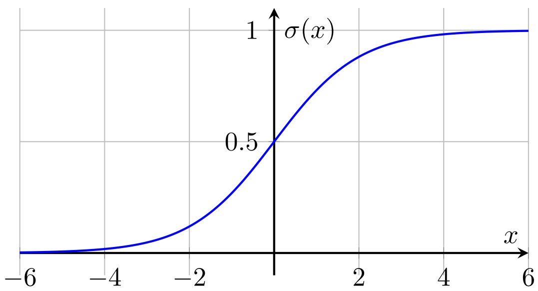

Figure 2.1: The sigmoid function $\sigma(z)$ over the interval $z \in [-6, 6]$.

The sigmoid function enjoys several elegant properties.

Theorem 2.1

$$1 - \sigma(z) = \sigma(-z)$$

Proof This follows directly from the definition of $\sigma(z)$, or equivalently, by observing the symmetry of its graph.

To convert soft prediction results into binary outputs $\{0, 1\}$, we introduce a threshold: when $\sigma(z) = 0.5$, the model makes a hard prediction.

Definition 2.2 (Separating Hyperplane)

The condition $\sigma(z) = 0.5$ defines the separating hyperplane. *It partitions the input space $\mathbb{R}^d$ into two regions, thereby transforming probabilistic predictions into binary classification outcomes.*

The normal vector w is perpendicular to this hyperplane and points towards the region where the model predicts class 1 (i.e., where $p(y = 1 \mid x) > 0.5$). We ensure this property by choosing the orientation of w accordingly.

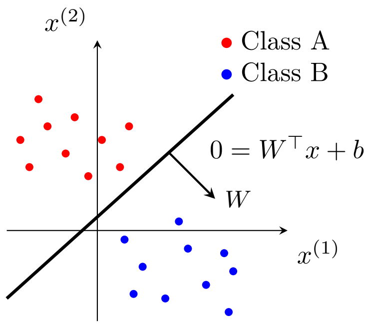

Figure 2.2: Classification by heperplane.

Model definition is clear, and now we turn our attention to parameter optimization. The question is: how can we find the proper w, b that achieve the best performance? The key problem here is to identify a suitable loss function that can be optimized via gradient descent.

Notice that:

$$P(y = 1 \mid x = x_i) = \sigma(f(x_i)) = \frac{1}{1 + \exp(-w^\top x + b)}. \tag{2.2}$$

We introduce a new method rather than continuing with ERM, by using **Maximum Likelihood Estimation (MLE)**. MLE is naturally designed to address probability modeling problems.

Definition 2.3 (Maximum Likelihood Estimation (MLE))

MLE aims to find parameters such that the likelihood of $P(y = y_i \mid x = x_i)$ is maximized. ♣

Remark For brevity, we write $P(y = y_i \mid x = x_i)$ as $P(y_i \mid x_i)$.

Definition 2.4 (Likelihood)

The likelihood on the entire training data is defined as

$$\prod_{i \in [n]} P(y_i \mid x_i; w, b) \tag{2.3}$$

assuming the samples are independent. ♣

According to the discussion above, in logistic regression we :

$$P(y_i \mid x_i) = \begin{cases} \sigma(w^\top x_i + b), & y_i = 1, \\ 1 - \sigma(w^\top x_i + b), & y_i = 0. \end{cases} \tag{2.4}$$

Therefore, the likelihood function can be expanded as:

$$\prod_{i \in [n]} \sigma(w^\top x_i + b)^{y_i} \left(1 - \sigma(w^\top x_i + b)\right)^{1 - y_i} \tag{2.5}$$

The above form is intuitive once we recall that $x^0 = 1$.

To ensure floating-point precision, given the large amount of data and the monotonicity of the logarithm function, we transform the likelihood into the maximization of the log-likelihood:

$$\operatorname*{argmax}_{w,b} \sum_{i \in [n]} \left[y_i \log \sigma(w^\top x_i + b) + (1 - y_i) \log \left(1 - \sigma(w^\top x_i + b)\right) \right] \tag{2.6}$$

This is the final objective in MLE.

MLE can be transformed into ERM by applying argmin to the negative log-likelihood. We define the **Cross-entropy**

Loss:

$$\mathcal{L}(w,b) := -\sum_{i\in[n]}\left[y_i \log\sigma(w^\top x_i + b) + (1-y_i)\log\left(1-\sigma(w^\top x_i + b)\right)\right] \tag{2.7}$$

Thus, minimizing the cross-entropy loss is equivalent to maximizing the log-likelihood, making the equivalence between MLE and ERM immediate

Note *Why is the above loss called the Cross-entropy loss? The name originates from information theory. Entropy is defined as:*

$$H(P) = \sum_y P(y)\log\frac{1}{P(y)} = -\sum_y P(y)\log P(y). \tag{2.8}$$

In other words, rarer events (with smaller probability) carry more information, and entropy measures the expected amount of information. In our context, we can evaluate the information content of the prediction for $y = \hat{y}_i$ given $x = x_i$ as:

$$\begin{aligned} H(P) &= -\sum_{\hat{y}_i\in\{0,1\}} P(y=\hat{y}_i \mid x_i)\,\log P(y=\hat{y}_i \mid x_i) \\ &= -[P(y=1\mid x_i)\,\log P(y=1\mid x_i) + P(y=0\mid x_i)\,\log P(y=0\mid x_i)] \end{aligned} \tag{2.9}$$

Notice that under our estimation, $P(y=1\mid x_i) = \sigma(f(x_i;w,b))$ and $P(y=0\mid x_i) = 1-\sigma(f(x_i;w,b))$. In practice, we substitute the empirical distribution of samples for the true distribution when comparing the negative log-likelihood with entropy. This is why the terminology of entropy from information theory is carried over to name this loss term.

Note *The formal definition of cross entropy between two propbability distributions q and p $H(q,p)$ is defined by:*

$$H(q,p) = -\sum_y q(y)\log p(y) \tag{2.10}$$

Definition 2.5 (KL-Divergence)

The KL-Divergence between two distributions p and q is defined by:

$$\mathrm{KL}(q\|p) = \sum_y q(y)\log\frac{q(y)}{p(y)} \tag{2.11}$$

♣

KL-Divergence measures the difference between two given distributions. In particular, $\mathrm{KL}(q\|p)$ differs from the cross-entropy by only a constant term $H(q)$:

$$\mathrm{KL}(q\|p) = H(q,p) - H(q). \tag{2.12}$$

In other words, KL-Divergence quantifies the extra number of bits required when we use p to approximate the ground-truth distribution q.

Back to the main content. Recall that a closed-form solution can be derived for the linear regression problem, as mentioned in the previous chapter. Here, we would like to investigate whether logistic regression also admits a closed-form solution.

Following the same steps we applied in linear case, we define $\hat{x} = (x^\top, 1)^\top \in \mathbb{R}^{d+1}$ and $\hat{w} = (w^\top, b)^\top \in \mathbb{R}^{d+1}$, thus $f(x) = \hat{w}^\top\hat{x}$:

$$\begin{aligned} \mathcal{L}(\hat{w}) &= -\sum_{i\in[n]} y_i\log\sigma(\hat{w}\hat{x}_i) + (1-y_i)\log(1-\sigma(\hat{w}^\top\hat{x}_i)) \\ &= -\sum_{i\in[n]} y_i\log\frac{1+\exp(\hat{w}^\top\hat{x}_i)}{1+\exp(-\hat{w}^\top\hat{x}_i)} - \log(1+\exp(\hat{w}^\top\hat{x}_i)) \\ &= -\sum_{i\in[n]} y_i(\hat{w}^\top\hat{x}_i) - \log(1+\exp(\hat{w}^\top\hat{x}_i)) \end{aligned} \tag{2.13}$$

Take the derivative:

$$\frac{\partial \mathcal{L}(\hat{w})}{\partial \hat{w}} = -\sum_{i\in[n]}\left[y_i\hat{x}_i - \frac{\exp(\hat{w}^\top\hat{x}_i)}{1+\exp(\hat{w}^\top\hat{x}_i)}\hat{x}_i\right] \tag{2.14}$$

$$= -\sum_{i\in[n]}\left[y_i - P(y=1\mid x_i)\right]\hat{x}_i \tag{2.15}$$

By gradient descent, the parameter is updated as $\hat{w} \leftarrow \hat{w} + \alpha\sum_{i\in[n]}\left(y_i - P(y_i=1\mid x_i)\right)\hat{x}_i$. This makes sense, since the term $y_i - P(y_i = 1 \mid x_i)$ directly measures the prediction error on sample i, and the update moves $\hat{w}$ a small step along the direction of the input $\hat{x}_i$ to reduce this error.

If for all i, we have $y_i = P(y=1\mid x_i)$, then the model predicts every label y_i perfectly. At this point, optimization reaches a stationary solution. If the training data admits such a perfect solution:

Definition 2.6 (linearly separable)

If all points can be separated by a linear model without error, we say the dataset is linearly separable. ♣

Example 2.3 is linearly separable, and the final state leads to $\|W\|\to\infty, \quad \|b\|\to\infty$. However, this situation is not desirable in practice, since it implies poor robustness. Hence a natural question arises: under the condition of linear separability, how can we find a well-chosen separating hyperplane that maximizes robustness? The answer will be presented in the next chapter, where we introduce the Support Vector Machine (SVM). The SVM optimizes $\hat{w}, \hat{b}$ by maximizing the margin (the distance between data points and the separating hyperplane), instead of simply minimizing the cross-entropy loss.

Although logistic regression may suffer from divergence of parameters under separable data, it often achieves better performance than SVM in practice, due to the following reasons:

1. In most real-world problems, the data are not linearly separable;
2. Applying L_2 regularization can effectively prevent parameter divergence.

Remark Why can't we use squared loss for classification? The reason is that in classification tasks such as logistic regression, the label $y \in \{0,1\}$ should be interpreted as a categorical outcome rather than a numerical quantity.

Example 2.2 Multi-Class Classificaiton (Softmax Regression)

We can combine k sub-classifiers to solve a k-class classification task. Specifically, we apply a sigmoid-like transformation to each sub-linear model $f_k(x) = w_k^\top x + b_k$, and obtain the probability of class k using a normalized expression:

$$P(y=k\mid x) = \frac{\exp(w_k^\top x + b_k)}{\sum_{j=1}^{k}\exp(w_j^\top x + b_j)}. \tag{2.16}$$

Note *There is a close analogy between* ***softmax regression*** *in machine learning and the* ***partition function*** *in statistical physics.*

In softmax regression, the probability of assigning an input x to class k is

$$P(y=k\mid x) = \frac{\exp(\theta_k^\top x)}{\sum_{j=1}^{K}\exp(\theta_j^\top x)}. \tag{2.17}$$

Here the denominator

$$Z(x) = \sum_{j=1}^{K}\exp(\theta_j^\top x) \tag{2.18}$$

serves as a normalizing constant*, ensuring that the probabilities over all classes sum to* 1.

In statistical physics, for a system with possible states s of energy $E(s)$, the probability of observing state s under the Boltzmann distribution is

$$P(s) = \frac{\exp(-\beta E(s))}{Z} = -\frac{1}{\beta}\frac{\partial \log Z}{\partial E(s)}, \quad Z = \sum_s \exp(-\beta E(s)), \tag{2.19}$$

where Z is the partition function*. It normalizes the distribution and encodes all thermodynamic properties of the system.*

Thus, the role of $Z(x)$ in softmax regression is mathematically analogous to the role of the partition function Z in *statistical physics: both are log-sum-exp normalizers that transform unnormalized scores (energies or logits) into proper probability distributions.*

The softmax regression method has several advantages:

1. It is unified and normalized: $\sum_{j\in[j]} P(y = k \mid x) = 1$;
2. The amplify effect of exp function: when $f_k(x) \gg f_j(x), \forall j \neq k$, then $P(y = k \mid x) = 1$.

We apply the same MLE procedure to the multi-class classification task, which leads to the following optimization problem:

$$\underset{\{w_k,b_k\}}{\operatorname{argmax}} \sum_{i\in[n]} \log \frac{\exp(w_k^\top x_i + b_k)}{\sum_{j=1}^{k} \exp(w_j^\top x_i + b_j)} \tag{2.20}$$

Note *In modern neural networks, softmax regression is widely used as the standard classification method.*

Remark When $k = 2$, softmax regression reduces to logistic regression via the reparameterization $w = w_1 - w_2$ and $b = b_1 - b_2$.

Example 2.3 MLE Explanation for Linear Regression

Definition 2.7 (Gaussian/Normal Distribution)

$$x \sim \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{2.21}$$

♣

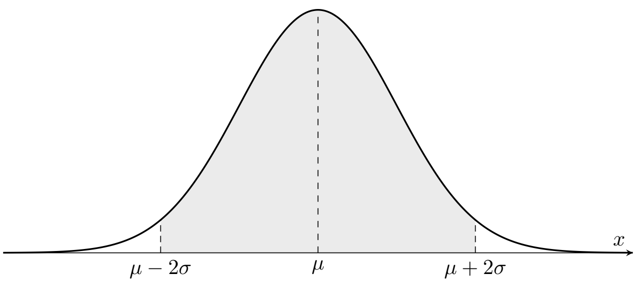

Figure 2.3: Normal distribution (95%).

While the Central Limit Theorem (CLT) does not imply that most datasets are normally distributed, it motivates modeling additive noise as Gaussian. We assume:

$$y = \underbrace{w^\top x + b}_{\text{latent model}} + \underbrace{\varepsilon}_{\text{noise}}, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2) \tag{2.22}$$

where σ^2 is a hyperparameter characterizing the noise scale. Then:

$$P(y \mid x; w, b, \sigma^2) = \mathcal{N}\big(y \,\big|\, w^\top x + b,\ \sigma^2\big) \tag{2.23}$$

The log-likelihood takes the form:

$$\begin{aligned} \underset{w,b}{\operatorname{argmax}} \sum_{i\in[n]} \log \mathcal{N}\big(y_i \,\big|\, w^\top x_i + b,\ \sigma^2\big) &= \underset{w,b}{\operatorname{argmax}} \sum_{i\in[n]} \left[-\tfrac{1}{2}\log(2\pi\sigma^2) - \frac{\big(y_i - (w^\top x_i + b)\big)^2}{2\sigma^2}\right] \\ &\Leftrightarrow \underset{w,b}{\operatorname{argmin}} \sum_{i\in[n]} \big(y_i - (w^\top x_i + b)\big)^2, \end{aligned} \tag{2.24}$$

where the equivalence follows by dropping constants and positive scalings. Equation (2.24) recovers ERM with the squared-loss objective.

Example 2.4 Maximum a Posteriori (MAP)

In the MLE perspective, w and b are treated as unknown fixed constants. In the Bayesian framework, however, even w, b are considered as random variables (R.V.). A "fixed constant" can be seen as a random variable with an extremely sharp distribution (near δ-distribution).

Suppose we place a Gaussian prior $P(\hat{w}) = \mathcal{N}(\hat{w} \mid 0,\ \sigma_w^2 \mathbb{I})$. The likelihood is given by

$$P(y \mid x, \hat{w};\, \sigma^2, \sigma_w^2) = \mathcal{N}\big(y \mid \hat{w}^\top \hat{x},\ \sigma^2\big) \tag{2.25}$$

We want to compute the posterior distribution of $\hat{w}$. By Bayes' rule:

$$\begin{aligned} P(\hat{w} \mid y, x) &= \frac{P(y \mid x, \hat{w})\, P(\hat{w})}{P(y \mid x)} \\ &\propto \left(\prod_{i \in [n]} P(y_i \mid x_i, \hat{w}) \right) P(\hat{w}) \end{aligned}$$

Expanding this expression:

$$P(\hat{w} \mid y, x) = \frac{1}{Z} \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right)^n \exp\!\left(-\frac{1}{2\sigma^2} \sum_{i \in [n]} \big(y_i - \hat{w}^\top \hat{x}_i\big)^2 \right) \left(\frac{1}{\sqrt{2\pi\sigma_w^2}} \right)^{d+1} \exp\!\left(-\frac{\hat{w}^\top \hat{w}}{2\sigma_w^2} \right)$$

Taking the negative logarithm of the posterior, note that only the terms involving $\hat{w}$ are subject to optimization:

$$-\log P(\hat{w} \mid y, x) = \sum_{i \in [n]} \big(y_i - \hat{w}^\top \hat{x}_i\big)^2 + \frac{\sigma^2}{\sigma_w^2} \|\hat{w}\|^2 + \text{Const.}$$

Letting $\lambda = \sigma^2 / \sigma_w^2$, the MAP estimator is obtained by:

$$\operatorname*{argmin}_{\hat{w}} \sum_{i \in [n]} \big(y_i - \hat{w}^\top \hat{x}_i\big)^2 + \lambda \|\hat{w}\|^2, \tag{2.26}$$

which is exactly ridge regression. Therefore, the internal consistency of the theory is demonstrated.