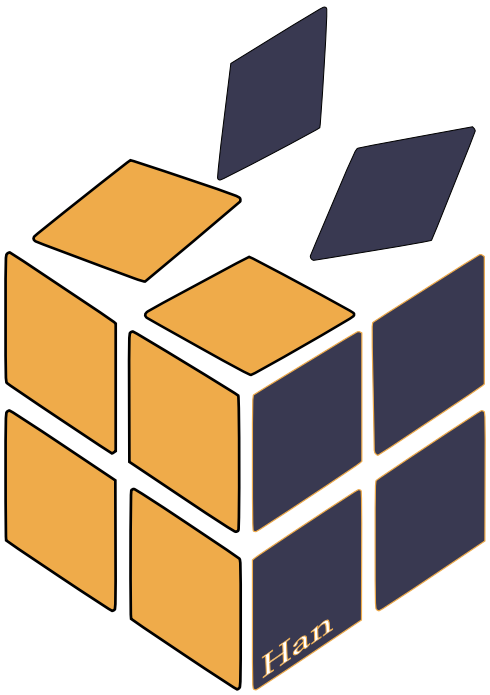
Deep Statistical Learning



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The logo depicts a cube puzzle gradually coming together, reflecting the journey of learning. Each piece represents a fragment of knowledge, and as they fall into place, they reveal the larger structure of understanding. It conveys the idea that growth is a process — knowledge is completed bit by bit.

Contents

Part I

Introduction

Chapter 1

Basics

1.1 Naive Bayes

Let's say we have a prediction model and it gives us a prediction. We want to measure the precision of the prediction. For example, the prediction has 90% chance of being a correct prediction. This can be modeled probabilistically. Given data $\mathbf{x}$, we want to know the probability of it being y. Similarly, if we have N data, then with an i.i.d., assumption,

$$\prod_{i=1}^{N} p(y_i|\mathbf{x}_i).$$

What we want to is to build such a probabilistic model parameterized by some parameters.

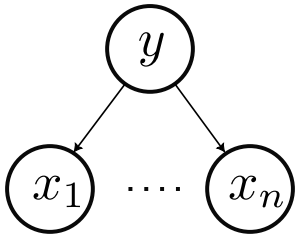
In this section, we discuss how to classify vectors of discrete-valued features $\mathbf{x}$. Recall that we discussed how to classify a feature vector $\mathbf{x}$ by applying Bayes rule to a generative classifier of the form

$$p(y = c|\mathbf{x}, \boldsymbol{\theta}) \propto p(\mathbf{x}|y = c, \boldsymbol{\theta})p(y = c|\boldsymbol{\theta})$$

The key to using such models is specifying a suitable form for the class-conditional density $p(\mathbf{x}|y = c, \boldsymbol{\theta})$, which defines what kind of data we expect to see in each class.

- $\mathbf{x} \in \{1, ..., K\}^D$,
  - K: the number of values for each feature.
  - D: the number of features.
- We will use a generative approach.
- Need to specify the class conditional distribution, $p(\mathbf{x}|y = c)$.
- A simple approach is to assume the features are **conditionally independence** given the class label.
- This allows us to write the class conditional density as a product of one dimensional densities:

$$p(\mathbf{x}|y = c, \boldsymbol{\theta}) = \prod_{j=1}^{D} p(x_j|y = c, \boldsymbol{\theta}_{jc})$$



The resulting model is called a **naive Bayes classifier (NBC)**. The model is called "naive" since we assume the independence between the features, which is not true in practice. However, if often results in classifiers that work well.

The form of the class-conditional density depends on the type of each feature. We give some possibilities below:

- In the case of real-valued features, we can use the Gaussian distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \mathcal{N}(x_j|\mu_{jc}^2)$, where μ_{jc} is the mean of feature j in objects of class c, and σ_{jc}^2 is its variance.
- In the case of binary features, we can use the Bernoulli distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \text{Ber}(x_j|\mu_{jc})$, where μ_{jc} is the probability that feature j occurs in class c. This is sometimes called the **multivariate Bernoulli naive Bayes** model.
- In the case of categorical features, $x_j \in \{1,...,K\}$, we can model the multinomial distribution: $p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \text{Cat}(x_j|\mu_{jc})$, where $\boldsymbol{\mu}_{jc}$ is a histogram over the K possible values for x_j in class c.

The probability for a single data case is given by

$$p(\mathbf{x}_i, y_i|\boldsymbol{\theta}) = p(y_i|\boldsymbol{\pi}) \prod_j p(x_{ij}|\boldsymbol{\theta}_j) = \prod_c \pi_c^{\mathbb{I}(y_i=c)} \prod_j \prod_c p(x_{ij}|\boldsymbol{\theta}_{jc})^{\mathbb{I}(y_i=c)},$$

where $\boldsymbol{\pi}$ is a vector of class probability. Hence the log-likelihood is given by

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{j=1}^{D} \sum_{c=1}^{C} \sum_{i:y_i=c} \log p(x_{ij}|\boldsymbol{\theta}_{jc})$$

Algorithm 1: Fitting a naive Bayes classifier to binary features

```
Initialize N_c = 0, N_jc = 0 ;
for i = 1 : N do
    c = y_i //Class label of i-th example;
    N_c := N_c + 1;
    for j = 1 : D do
        if x_ij = 1 then
            N_jc := N_jc + 1
    end
end
```

$\hat{\pi} = \frac{N_c}{N}, \hat{\theta}_{jc} = \frac{N_{jc}}{N_c}$

Chapter 2

Evaluation Metrics

2.1 Basic Metrics

2.1.1 Confusion matrix

	Predicted		
Actual		T	N
	T	TP	FN
	N	FP	TN

Some special metrics:

- **Recall** (or **TPR**): Find all relevant cases whithin a dataset.

$$\frac{TP}{TP + FN}$$

- **Precision**: While recall expresses the ability to find all relevant instances in a dataset, precision expresses the proportion of the data points our model says was relevant actually were relevant.

$$\frac{TP}{TP + FP}$$

- **FPR**: the percentage of actual Negatives that were incorrectly classified.

$$\frac{FP}{FP + TN}$$

2.1.2 Receiver Operating Characteristic (ROC)

ROC curves are helpful when we need to identify how well each threshold performed in terms of the TPR and the FPR of binary classifier. *ROC* stands for *Receiver Operating Characteristic*, and the name comes from the graphs drawn during World War II that summarized how well radar operators correctly identified airplanes in radar signals. The illustrative ROC curve is given as follows:

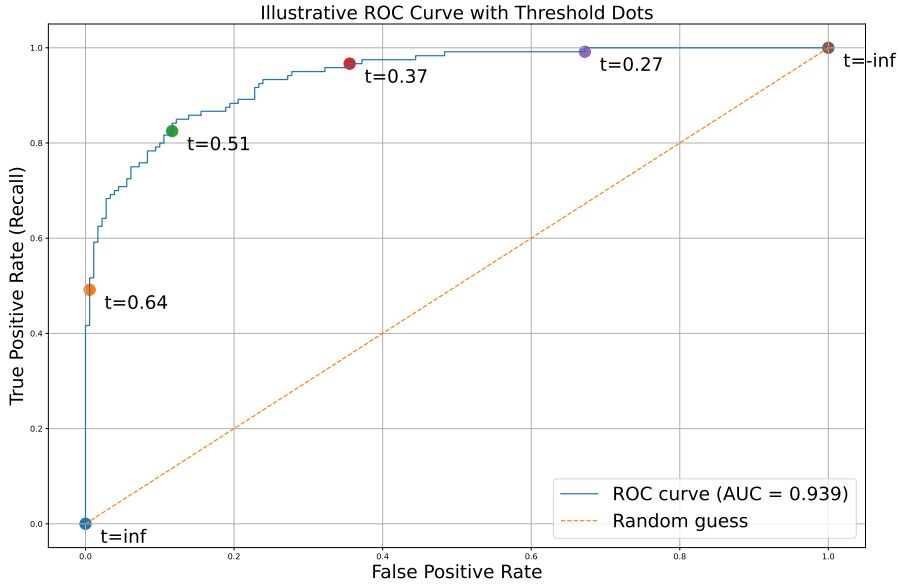


Figure 2.1: Each dot on the ROC curve represents the TPR and the FPR at a specific threshold.

- The diagonal line shows where the TRP = FPR.
- A point near $(0, 1)$ is ideal: low false alarms, high detection.
- Higher curve = better. The AUC (area under the ROC) summarizes performance across all thresholds (1.0 is perfect). AUC is especially helpful when we have to compare multiple models, since it provides a simple comparison.
- Choose the point that best matches your costs/requirements.

2.1.3 Precision Recall Graphs

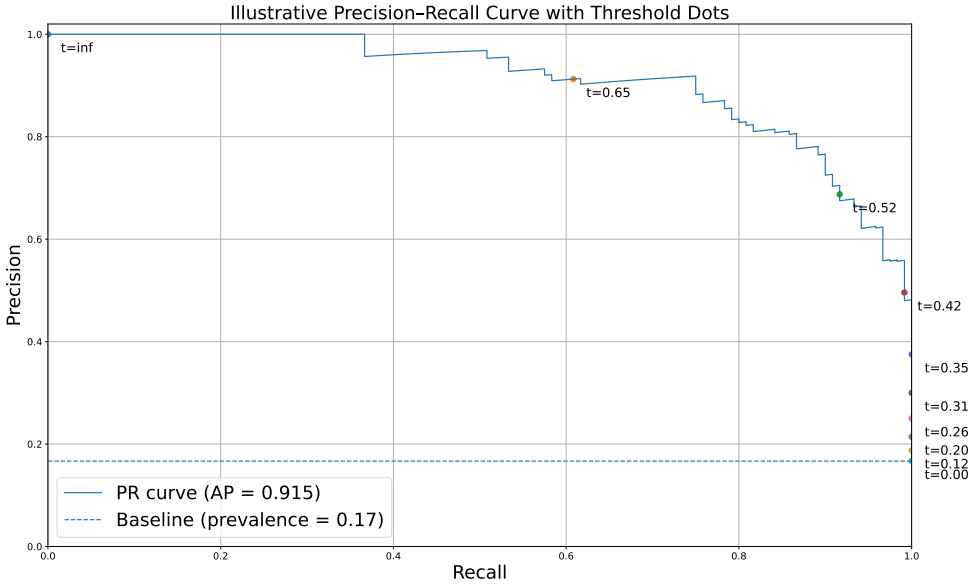
When classes are highly imbalanced, ROC curves can be misleading. With very few positives, the false positive rate (FPR) can stay low even for weak models, giving an overly optimistic picture. In these cases, precision–recall (PR) curves are more informative because they focus on the positive class: they plot precision (y-axis) versus recall (x-axis), where recall equals TPR. PR curves highlight how many of the predicted positives are actually correct (precision) at each level of coverage (recall), making them better suited for rare-event detection.

This is because precision is more informative than FPR under heavy class imbalance: precision ignores true negatives (TN), whereas FPR uses them. The illustrative plot below shows the difference.

In sum, for imbalanced data, use PR curves (precision vs recall) instead of ROC: FPR can look small simply because true negatives dominate, while PR directly measures the quality of positive predictions.

Rule of thumbs:

- For rare positives or alerting workflows: use PR (and report precision@recall or re-



call@precision).

- For balanced data or TN-sensitive views: also show ROC/AUC.

Chapter 3

Dimensionality Reduction

3.1 Principal Component Analysis

3.1.1 Covariance and the weight vector

When deriving PCA, we seek a vector $\mathbf{w}$ (the weight vector or loading vector) such that the projection of the data onto this vector maximizes the variance. Maximizing the variance is equivalent to projecting the data onto a lower-dimensional linear subspace in such a way that the distance between a vector and its projection is not too large. For a given data matrix $\mathbf{X}$ with mean zero (mean-centered data), the projection of the data onto $\mathbf{w}$ is given by $\mathbf{Xw}$.

In other words, PCA aims to find the most accurate data representation in a lower dimensional space spanned by the maximum-variance directions.

The variance of the projected data can be expressed as:

$$\mathrm{Var}(\mathbf{Xw}) = \frac{1}{n}(\mathbf{Xw})^T(\mathbf{Xw}) = \frac{1}{n}\mathbf{w}^T\mathbf{X}^T\mathbf{Xw}$$

Where n is the number of data points. The matrix $\mathbf{X}^T\mathbf{X}$ is the covariance matrix of the data (up to a scaling factor).

The goal is to maximize the variance $\mathbf{w}^T\mathbf{X}^T\mathbf{Xw}$ with respect to the weight vector $\mathbf{w}$, subject to the constraint that $\mathbf{w}^T\mathbf{w} = 1$ (to prevent the trivial solution where the variance could be made arbitrarily large just by scaling $\mathbf{w}$).

$$\mathcal{L} = \frac{1}{n}\mathbf{w}^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{Xw} - \lambda\left(\mathbf{w}^\mathsf{T}\mathbf{w} - 1\right)$$

$$\frac{\partial\mathcal{L}}{\partial\mathbf{w}} = \frac{2}{n}\mathbf{X}^\mathsf{T}\mathbf{Xw} - 2\lambda\mathbf{w} = \mathbf{0}$$

$$\underbrace{\frac{1}{n}\mathbf{X}^\mathsf{T}\mathbf{X}}_{:=\mathbf{S}}\mathbf{w} = \lambda\mathbf{w} \quad \Rightarrow \quad \mathbf{Sw} = \lambda\mathbf{w}$$

This is exactly the eigenvalue equation. The eigenvectors $\mathbf{w}$ are the directions that maximize the variance, and the eigenvalues λ represent the magnitude of the variance along those directions.

- Eigenvectors: Each eigenvector of the covariance matrix represents a direction in the feature space. These directions are the principal components.
- Eigenvalues: The corresponding eigenvalue tells us how much variance is captured along that direction. The larger the eigenvalue, the more variance is captured by the corresponding eigenvector.

$$\text{Var}(\mathbf{Xw}) = \frac{1}{n}(\mathbf{Xw})^T(\mathbf{Xw}) = \frac{1}{n}\mathbf{w}^T\mathbf{X}^T\mathbf{Xw} = \frac{1}{n}\mathbf{w}^T\mathbf{Sw} = \frac{1}{n}\mathbf{w}^T\lambda\mathbf{w} = \frac{1}{n}\lambda$$

Capturing the Most Information:

- Variance is a measure of how spread out the data is along a particular direction. By maximizing the variance, we ensure that the principal components capture the most significant patterns in the data.
- If we reduce the dimensionality by selecting components with the highest variance, we retain the most information about the data, effectively compressing the data without losing critical details.
- High variance indicates that the data points are spread out and less likely to be redundant. Conversely, low variance implies that data points are clustered close together, often making the information less significant.

Sort eigenvectors $v_1, v_2, \ldots, v_d$ in descending order of their corresponding eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$.

Then, select the first k eigenvectors to form a projection matrix:

$$W_k = [v_1, v_2, \ldots, v_k] \in \mathbb{R}^{d \times k}$$

Now project the centered data onto this new basis:

$$Z = X_{\text{centered}} W_k \in \mathbb{R}^{n \times k}$$

This gives the data in the lower-dimensional space.

3.2 Linear Discriminant Analysis

We seek to obtain a transformation of X to Y through projecting the samples in X onto a hyperplane.

- Data matrix $\mathbf{X} = \left[\mathbf{x}_1, \ldots, \mathbf{x}_N\right]^\top \in \mathbb{R}^{N \times m}$ with row-vectors $\mathbf{x}_i$.

- Class labels $i \in \{1, \ldots, C\}$, and each class has N_i samples.
- Each sample is belong to class ω_i.

Of all the possible lines we would like to select the one that maximizes the separability. In order to find a good projection vector, we need to define a measure of separation between the projections.

The mean vector of each class in $\mathbf{x}$ and $\mathbf{y}$ is given by

$$\mu_i = \frac{1}{N} \sum_{\mathbf{x} \in \omega_i} \mathbf{x}$$
$$\tilde{\mu}_i = \frac{1}{N} \sum_{\mathbf{y} \in \omega_i} \mathbf{y} = \frac{1}{N} \sum_{\mathbf{y} \in \omega_i} \mathbf{w}^T \mathbf{x} = \mathbf{w}^T \frac{1}{N} \sum_{\mathbf{y} \in \omega_i} \mathbf{x} = \mathbf{w}^T \mu_i$$

This indicates that projecting leads to projecting the mean of $\mathbf{x}$ to the mean of $\mathbf{y}$. Then, we could set the distance between the projected means as our objective function as follows:

$$J(\mathbf{w}) = |\tilde{\mu}_1 - \tilde{\mu}_2| = |\mathbf{w}^T(\mu_1 - \mu_2)|.$$

However, maximizing the distance between the projected means is not enough to yield better class separability. Thus, we will introduce the within-class variability, so-called *scatter* matrix:

$$S_i = \sum_{\mathbf{x} \in \omega_i} (\mathbf{x} - \mu_i)(\mathbf{x} - \mu_i)^T$$
$$S_W = S_1 + S_2$$

Where S_i is the covariance matrix of class ω_i, and S_ω is called the *within-class scatter matrix*.

Now the scatter of the projection $\mathbf{y}$ can then be expressed as a function of the scatter matrix in feature space $\mathbf{x}$.

$$\begin{aligned}
\tilde{s}_i^2 = \sum_{y \in \omega_i} (y - \mu_i)^2 &= \sum_{\mathbf{x} \in \omega_i} (w^T \mathbf{x} - w^T \mu_i)^2 \\
&= \sum_{\mathbf{x} \in \omega_i} \left(w^T (\mathbf{x} - \mu_i) \right)^2 \\
&= \sum_{\mathbf{x} \in \omega_i} \underbrace{\left(w^T (\mathbf{x} - \mu_i) \right)}_{scalar} \underbrace{\left(w^T (\mathbf{x} - \mu_i) \right)}_{scalar^T = scalar} \\
&= \sum_{\mathbf{x} \in \omega_i} w^T (\mathbf{x} - \mu_i)(\mathbf{x} - \mu_i)^T w \\
&= w^T S_i w.
\end{aligned}$$

Thus,

$$\tilde{s}_1^2 + \tilde{s}_2^2 = w^T S_1 w + w^T S_2 w = w^T (S_1 + S_2) w = w^T S_W w = \tilde{S}_W.$$

Similarly, the difference between the projected means can be expressed as follows:

$$\begin{aligned}
(\tilde{\mu}_1 - \tilde{\mu}_2)^2 &= (w^T \mu_1 - w^T \mu_2) \\
&= w^T (\mu_1 - \mu_2)(\mu_1 - \mu_2)^T w \\
&= w^T S_B w = \tilde{S}_B
\end{aligned}$$

This matrix is called the *between-class scatter*. Since S_B is the outer product of two vectors, its rank is at most one.

For a projection vector $\mathbf{w} \in \mathbb{R}^d$ (with $\mathbf{w} \neq \mathbf{0}$) define the *Fisher ratio*

$$J(\mathbf{w}) = \frac{|\tilde{\mu}_1 - \tilde{\mu}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2} = \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}.$$

The optimal w satisfies that $|\tilde{\mu}_1 - \tilde{\mu}_2|$ (inter-class spread) is big and $\tilde{s}_1^2 + \tilde{s}_2^2$ (intra-class spread) is small. Note that this objective function is called *Rayleigh quotient*.

Maximising the objective J with respect to $\mathbf{w}$ is equivalent to maximising the numerator while holding the denominator constant as both the numerator and denominator have the same order of $\|\mathbf{w}\|$ and thus J is invariant to scale changes in $\|\mathbf{w}\|$. Further, as we are only interested in the direction of $\mathbf{w}$, we can hold the denominator constant to 1. This results in a Lagrangian:

$$\mathcal{L}(\mathbf{w}, \lambda) = \mathbf{w}^\top S_B \mathbf{w} - \lambda(\mathbf{w}^\top S_W \mathbf{w} - 1).$$

- If you scale $\mathbf{w}$ by any nonzero scalar c, then numerator: $(c\mathbf{w})^\top S_B (c\mathbf{w}) = c^2\, \mathbf{w}^\top S_B \mathbf{w}$ denominator: $(c\mathbf{w})^\top S_W (c\mathbf{w}) = c^2\, \mathbf{w}^\top S_W \mathbf{w}$. The factor c^2 cancels in the ratio, so $J(c\mathbf{w}) = J(\mathbf{w})$. Therefore, only the direction of $\mathbf{w}$ matters, not its length. That's what invariant to scale changes in $\|\mathbf{w}\|$ means.
- Because the ratio is scale-invariant, we can arbitrarily fix the scale of $\mathbf{w}$. The common choice is: $\mathbf{w}^\top S_W \mathbf{w} - 1$.

Then, $\partial\mathcal{L}/\partial\mathbf{w} = \mathbf{0}$ gives

$$S_B \mathbf{w} = \lambda S_W \mathbf{w}.$$
$$S_W^{-1} S_B \mathbf{w} = \lambda \mathbf{w}.$$

By using the definition of S_B,

$$S_W^{-1} S_B \mathbf{w} = S_W^{-1} (\tilde{\mu}_1 - \tilde{\mu}_2)(\tilde{\mu}_1 - \tilde{\mu}_2)^T \mathbf{w} = \lambda \mathbf{w}.$$

Let's set $(\tilde{\mu}_1 - \tilde{\mu}_2)^T \mathbf{w} = \alpha$ and α is a scalar. Then, we get

$$S_W^{-1} (\tilde{\mu}_1 - \tilde{\mu}_2) = \frac{\lambda \mathbf{w}}{\alpha}$$

Since we are only interested in the direction of $\mathbf{w}$, we can discard the scalar term, then

$$\mathbf{w}^* = S_W^{-1} (\tilde{\mu}_1 - \tilde{\mu}_2).$$

Chapter 4

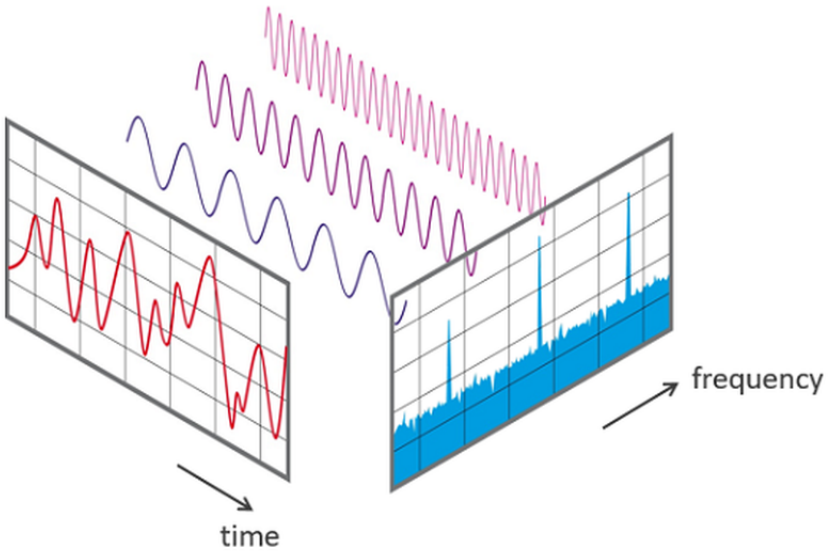
Fourier Analysis

Fourier analysis is a mathematical tool used to understand and analyze periodic phenomena. It is named after the French mathematician Joseph Fourier, it's based on the idea that any periodic function can be represented as a sum of sine and cosine functions with different frequencies, amplitudes, and phases.

The Fourier transform is one of the most important mathematical tools used for analyzing functions. Given an arbitrary function $f(x)$, with a real domain ($x \in \mathbb{R}$), we can express it as a linear combination of complex waves ($\approx$ change of basis to a frequency domain).

- Periodic Functions: Fourier analysis deals with functions that repeat over regular intervals. This repetition could be over time (like sound waves or electrical signals) or space (like patterns on a surface).
- Fourier Series: It states that any periodic function can be represented as an infinite sum of sine and cosine functions. The Fourier series expansion expresses the original function as a weighted sum of sinusoids.
- Frequency Domain: While the original function is in the time or spatial domain, Fourier analysis allows us to examine it in the frequency domain. This means we can understand the different frequency components present in the signal and their respective strengths.
- Fast Fourier Transform (FFT): This is an efficient algorithm for calculating the Fourier transform of a discrete signal. It's widely used in digital signal processing due to its speed and accuracy.
- Continuous vs. Discrete Fourier Transform: While Fourier series deals with periodic continuous functions, Fourier transforms extend the concept to non-periodic functions or signals. The discrete Fourier transform (DFT) is used for discrete, sampled signals, as in digital signal processing.
- Inverse Fourier Transform: Just as you can transform a function into the frequency domain using Fourier analysis, you can also transform it back using the inverse Fourier transform. This allows you to reconstruct the original function from its frequency components.

Very intuitive explanation is here!



4.1 Fourier Series

We begin by discussing the Fourier series, which is used to analyze functions that are periodic in their inputs. A periodic function $f(x)$ is a function of a real variable x that repeats itself every time x changes by T. The constant T is called the *period*. We can write the periodicity condition as

$$f(x+T) = f(x), \forall x \in \mathbb{R}.$$

The value of $f(x)$ can be real or complex, but x should be real.

Let's consider what it means to specify a periodic function $f(x)$. One way to specify the function is to give an explicit mathematical formula for it. Another approach might be to specify the function values in $-T/2 \leq x < T/2$. Since there's an uncountably infinite number of points in this domain, we can generally only achieve an approximate specification of f this way, by giving the values of f at a large but finite set x points.

There is another interesting approach to specifying f. We can express it as a linear combination of simpler periodic functions, consisting of sines and cosines:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n x}{T}\right) + \sum_{m=1}^{\infty} b_m \sin\left(\frac{2\pi m x}{T}\right), \tag{4.1}$$

where a_0, a_n, and b_m are coefficients determined by integrating $f(x)$ over one period. The coefficients are given by

$$\begin{aligned} a_0 &= \frac{1}{T}\int_0^T f(x)dx \\ a_n &= \frac{2}{T}\int_0^T f(x)\cos\left(\frac{2\pi n x}{T}\right)dx \\ b_m &= \frac{2}{T}\int_0^T f(x)\sin\left(\frac{2\pi n x}{T}\right)dx \end{aligned}$$

The above formula is called a *Fourier series*. Given the numbers $\{a_n, b_m\}$, which are called the *Fourier coefficients*, $f(x)$ can be calculated for any x. The Fourier coefficients are real if $f(x)$ is a real function, or complex if $f(x)$ is complex.

Example: Consider a periodic function $f(x)$ defined on the interval $-\pi \leq x \leq \pi$ as follows:

$$f(x) = \begin{cases} 0 & \text{if } -\pi \leq x < 0 \\ x & \text{if } 0 \leq x \leq \pi \end{cases}$$

We want to find the Fourier series representation of $f(x)$.

Solution: Step 1: Determine the coefficients a_0, a_n, and b_n.

1. Calculate a_0:

$$\begin{aligned} a_0 &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx \\ &= \frac{1}{\pi} \left(\int_{-\pi}^{0} 0 \, dx + \int_{0}^{\pi} x \, dx \right) \\ &= \frac{1}{\pi} \left(\int_{0}^{\pi} x \, dx \right) \\ &= \frac{1}{\pi} \left(\frac{1}{2} \pi^2 \right) \\ &= \frac{\pi}{2} \end{aligned}$$

2. Calculate a_n:

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) \, dx$$

Since $f(x)$ is odd and $\cos(nx)$ is even, a_n will be zero for all n.

3. Calculate b_n:

$$\begin{aligned} b_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(nx) \, dx \\ &= \frac{1}{\pi} \left(\int_{0}^{\pi} x \sin(nx) \, dx \right) \end{aligned}$$

This integral can be evaluated using integration by parts:

$$u = x, \quad dv = \sin(nx) \, dx$$

$$du = dx, \quad v = -\frac{1}{n} \cos(nx)$$

$$\begin{aligned} b_n &= \frac{1}{\pi} \left(\left[-\frac{x}{n} \cos(nx) \right]_0^{\pi} - \frac{1}{n} \int_{0}^{\pi} -\cos(nx) \, dx \right) \\ &= \frac{1}{\pi} \left(\frac{\pi}{n} - \frac{1}{n^2} \left[\sin(nx) \right]_0^{\pi} \right) \\ &= \frac{1}{\pi} \left(\frac{\pi}{n} \right) \\ &= \frac{1}{n} \end{aligned}$$

4. Write the Fourier series:

$$f(x) = \frac{\pi}{2} + \sum_{n=1}^{\infty} \frac{1}{n} \sin(nx)$$

4.1.1 Square-integrable functions

Can arbitrary periodic functions always be expressed as a Fourier series? It turns out that a certain class of periodic functions, commonly encountered in physical contexts, are guaranteed to always be expressible as Fourier series. These are called square-integrable functions such that the integral of the square of the absolute value is finite:

$$\int_{-a/2}^{a/2} |f(x)|^2 dx < \infty.$$

Unless otherwise stated, we will always assume that the functions we're dealing with are square-integrable.

4.1.2 Complex Fourier series and inverse relations

We have written the Fourier series as a sum of sine and cosine functions. However, sines and cosines can be expressed by exponential functions by using *Euler's formula*.

$$e^{ix} = \cos x + i \sin x \tag{4.2}$$

- $\cos x = \frac{e^{ix}+e^{-ix}}{2}$
- $\sin x = \frac{e^{ix}-e^{-ix}}{2i}$

Thus, Fourier series can be expressed as follows:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx},$$

where the complex Fourier coefficients c_n are given by:

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx}\, dx$$

- i: complex number
- n: integer

Example: Consider the periodic function $f(x)$ defined on the interval $-\pi \leq x \leq \pi$:

$$f(x) = \begin{cases} 0 & \text{if } -\pi \leq x < 0 \\ x & \text{if } 0 \leq x \leq \pi \end{cases}$$

We will find the complex form of the Fourier series for this function.

Step 1: Calculate the complex Fourier coefficients c_n.

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx}\, dx$$

Since $f(x)$ is piecewise, we split the integral into two parts:

$$c_n = \frac{1}{2\pi}\left(\int_{-\pi}^{0} 0 \cdot e^{-inx}\,dx + \int_{0}^{\pi} xe^{-inx}\,dx\right)$$

The first integral is zero, so we focus on the second part:

$$c_n = \frac{1}{2\pi}\int_{0}^{\pi} xe^{-inx}\,dx$$

This integral can be solved using integration by parts. Let:

$$u = x \quad \text{and} \quad dv = e^{-inx}\,dx$$

Then:

$$du = dx \quad \text{and} \quad v = \frac{e^{-inx}}{-in} = -\frac{1}{in}e^{-inx}$$

Applying integration by parts:

$$\int u\,dv = uv - \int v\,du$$

So,

$$\int_{0}^{\pi} xe^{-inx}\,dx = \left[-\frac{x}{in}e^{-inx}\right]_{0}^{\pi} + \frac{1}{in}\int_{0}^{\pi} e^{-inx}\,dx$$

Evaluating the boundary terms:

$$\left[-\frac{x}{in}e^{-inx}\right]_{0}^{\pi} = -\frac{\pi}{in}e^{-in\pi} - 0 = -\frac{\pi}{in}e^{-in\pi}$$

And for the integral:

$$\frac{1}{in}\int_{0}^{\pi} e^{-inx}\,dx = \frac{1}{in}\left[\frac{e^{-inx}}{-in}\right]_{0}^{\pi} = -\frac{1}{n^2}\left(e^{-in\pi} - 1\right)$$

Combining these results:

$$\int_{0}^{\pi} xe^{-inx}\,dx = -\frac{\pi}{in}e^{-in\pi} + \frac{1}{n^2}(1 - e^{-in\pi})$$

Thus, the Fourier coefficient c_n is:

$$c_n = \frac{1}{2\pi}\left(-\frac{\pi}{in}e^{-in\pi} + \frac{1}{n^2}(1 - e^{-in\pi})\right)$$
$$c_n = \frac{1}{2\pi}\left(-\frac{\pi}{in}(-1)^n + \frac{1}{n^2}(1 - (-1)^n)\right)$$

This expression simplifies to:

$$c_n = \frac{i(-1)^n}{2n} + \frac{1}{2\pi n^2}(1 - (-1)^n)$$

Step 2: Write the Complex Fourier Series:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx}$$

With c_n now calculated, you can substitute these coefficients back into the Fourier series expression to represent $f(x)$.

4.2 Fourier Transform

4.2.1 Fourier Series v.s. Fourier Transform

The Fourier series is used to represent periodic functions as a sum of sine and cosine functions. On the other hand, the Fourier transform extends the idea to non-periodic functions or signals. The Fourier transform of a function $f(t)$ is given by:

$$F(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}\,dt,$$

where $F(\omega)$ is the frequency domain representation of the signal $f(t)$ and $\omega = 2\pi f$, where f is a frequency.

4.2.2 Equations of Fourier Transform

The Fourier transform and its inverse are defined as follows:

- Fourier Transform:
$$F(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}\,dt$$
- Inverse Fourier Transform:
$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{i\omega t}\,d\omega$$

These equations show how a time-domain signal $f(t)$ can be transformed into its frequency-domain representation $F(\omega)$, and vice versa.

Example: The Fourier transform of a rectangular pulse. Define a rectangular pulse function $f(t)$ as:

$$f(t) = \begin{cases} 1 & \text{if } |t| \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

To find its Fourier transform $F(\omega)$:

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t}\, dt$$

Since $f(t)$ is non-zero only between $-\frac{1}{2}$ and $\frac{1}{2}$, the integral becomes:

$$F(\omega) = \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i\omega t}\, dt$$

This integral can be evaluated as:

$$F(\omega) = \left[\frac{e^{-i\omega t}}{-i\omega}\right]_{-\frac{1}{2}}^{\frac{1}{2}} = \frac{e^{-i\omega/2} - e^{i\omega/2}}{-i\omega} = \frac{2\sin(\omega/2)}{\omega}$$

Thus, the Fourier transform of the rectangular pulse is:

$$F(\omega) = \frac{\sin(\omega/2)}{\omega/2} = \text{sinc}\left(\frac{\omega}{2}\right)$$

where $\text{sinc}(x) = \frac{\sin(x)}{x}$.

4.3 Fourier Transform as a Change of Basis

A change of basis in linear algebra is a fundamental concept that involves transitioning from one coordinate system to another within a vector space. This can simplify calculations, provide deeper insights, or align with different geometric interpretations. Let's break down the concept with definitions and steps:

Fourier analysis is closely related to the concept of change of basis in linear algebra. In Fourier analysis, we are essentially changing the basis from the standard basis of functions (e.g., the time domain for signals) to a basis of sinusoidal functions (*e.g.,* the frequency domain). Here's how this relationship works:

The Fourier transform (both continuous and discrete versions) can be seen as a change of basis from the time domain to the frequency domain. When we apply the Fourier transform to a signal x(t)x(t), we express it as a linear combination of sinusoidal basis functions.

- Standard Basis in Time Domain: In the time domain, a signal or function can be represented as a sum of basis functions, which are typically δ functions (impulse functions) or other

simple functions like polynomial terms. For example, a discrete-time signal $x[n]$ can be considered in terms of standard basis vectors.

- Fourier Basis in Frequency Domain: In the frequency domain, the basis functions are complex exponentials or sinusoidal functions $e^{i\omega t}$ (where i is the imaginary unit and ω is the angular frequency). The Fourier transform decomposes a signal into a sum of these sinusoidal basis functions.

The Fourier transform (both continuous and discrete versions) can be seen as a change of basis from the time domain to the frequency domain. When we apply the Fourier transform to a signal $x(t)$, we express it as a linear combination of sinusoidal basis functions.

Continuous Fourier Transform: The continuous Fourier transform of a function $x(t)$ is given by:

$$X(f) = \int_{-\infty}^{\infty} x(t)e^{-i2\pi ft}\,dt$$

Here, $X(f)$ represents the coordinates of the function $x(t)$ in the new basis (frequency domain). The inverse Fourier transform reconstructs the original signal from its frequency domain representation:

$$x(t) = \int_{-\infty}^{\infty} X(f)e^{i2\pi ft}\,df$$

This process is analogous to converting coordinates from the new basis back to the original basis.

4.3.1 Change of Basis

- Vector Space: A collection of vectors where vector addition and scalar multiplication are defined and satisfy specific axioms.
- Basis: A set of linearly independent vectors that span the entire vector space. Every vector in the space can be uniquely represented as a linear combination of the basis vectors.
- Coordinate Vector: The representation of a vector in terms of the basis vectors, typically given as a column of coefficients.

Steps for Change of Basis:

1. Representing Vectors in Original Basis: Given a vector space V with a basis $B = \{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_n\}$, any vector $\mathbf{v}$ in V can be written as:

   $$\mathbf{v} = c_1\mathbf{b}_1 + c_2\mathbf{b}_2 + \cdots + c_n\mathbf{b}_n$$

   Here, $c_1, c_2, \ldots, c_n$ are the coordinates of $\mathbf{v}$ relative to basis B, often written as $[\mathbf{v}]_B$.

2. Defining the New Basis: Suppose we want to change to a new basis $B' = \{\mathbf{b}'_1, \mathbf{b}'_2, \ldots, \mathbf{b}'_n\}$. We need to express the original basis vectors in terms of the new basis vectors. Let:

   $$\mathbf{b}_i = a_{i1}\mathbf{b}'_1 + a_{i2}\mathbf{b}'_2 + \cdots + a_{in}\mathbf{b}'_n$$

   for $i = 1, 2, \ldots, n$.

3. Constructing the Change of Basis Matrix: The coefficients a_{ij} form the columns of the change of basis matrix P from B to B':

$$P = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

4. Converting Coordinates: To convert the coordinates of a vector $\mathbf{v}$ from the original basis B to the new basis B', we use the change of basis matrix P:

$$[\mathbf{v}]_{B'} = P^{-1}[\mathbf{v}]_B$$

where P^{-1} is the inverse of the change of basis matrix and $[\mathbf{v}]_B = (c_1, \ldots, c_n)$ is a coordinate vector.

Conversely, to convert coordinates from the new basis B' back to the original basis B, we use:

$$[\mathbf{v}]_B = P[\mathbf{v}]_{B'}$$

Example: Consider a vector space $\mathbb{R}^2$ with an original basis $B = \{\mathbf{b}_1, \mathbf{b}_2\}$ and a new basis $B' = \{\mathbf{b}'_1, \mathbf{b}'_2\}$. Let:

$$\mathbf{b}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ \mathbf{b}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

and

$$\mathbf{b}'_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \ \mathbf{b}'_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

To find the change of basis matrix P from B to B', express the original basis vectors in terms of B':

$$\mathbf{b}_1 = \frac{1}{2}\mathbf{b}'_1 + \frac{1}{2}\mathbf{b}'_2$$

$$\mathbf{b}_2 = \frac{1}{2}\mathbf{b}'_1 - \frac{1}{2}\mathbf{b}'_2$$

So, the change of basis matrix P is:

$$P = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix}$$

To convert a vector $\mathbf{v}$ with coordinates $[\mathbf{v}]_B = \begin{bmatrix} x \\ y \end{bmatrix}$ to the new basis B', we compute:

$$[\mathbf{v}]_{B'} = P^{-1}[\mathbf{v}]_B$$

And to revert to the original basis:

$$[\mathbf{v}]_B = P[\mathbf{v}]_{B'}$$

Chapter 5

Training, Testing, and Regularization

5.1 Sources of Error in ML

$$E_{out} \leq E_{ml} + \Omega$$

- E_{out}: estimation of error.
- E_{ml}: error from a learning algorithm
- Ω: error caused by the variance from observations.

We also define

- f: target function
- g: learning function
- $g^{(D)}$: learned function based on D, or simply *hypothesis*.
- D: dataset drawn from the real world.
- $\bar{g}$: the average hypothesis of a given infinite number of Ds.

$$\bar{g}(x) = \mathbb{E}_D[g^{(D)}(x)].$$

Error of a single instance x from g learnt from D is given by

$$Err_{\text{out}}(g^{(D)}(x)) = \mathbb{E}_X[(g^{(D)}(x) - f(x))^2],$$

where X can be considered as test sets. Then, the expected error over the infinite number of datasets D sampled from a true data distribution is

$$\begin{aligned}\mathbb{E}_D[Err_{\text{out}}(g^{(D)}(x))] &= \mathbb{E}_D[\mathbb{E}_X[(g^{(D)}(x) - f(x))^2]] \\ &= \mathbb{E}_X[\mathbb{E}_D[(g^{(D)}(x) - f(x))^2]]\end{aligned}$$

Let's simplify the term inside with an average of hypothesis $\bar{g}(x)$:

$$\begin{aligned}\mathbb{E}_D[(g^{(D)}(x) - f(x))^2] &= \mathbb{E}_D[(g^{(D)}(x) - \bar{g}(x) + \bar{g}(x) - f(x))^2] \\ &= \mathbb{E}_D\big[(g^{(D)}(x) - \bar{g}(x))^2 + (\bar{g}(x) - f(x))^2 \\ &\quad + 2(g^{(D)}(x) - \bar{g}(x))(\bar{g}(x) - f(x))\big] \\ &= \mathbb{E}_D\big[(g^{(D)}(x) - \bar{g}(x))^2\big] + (\bar{g}(x) - f(x))^2 \\ &\quad + \mathbb{E}_D\big[2(g^{(D)}(x) - \bar{g}(x))(\bar{g}(x) - f(x))\big]\end{aligned}$$

Since, $\mathbb{E}_D\big[2(g^{(D)}(x) - \bar{g}(x))(\bar{g}(x) - f(x))\big]$ is 0, the expectation of the error becomes

$$\mathbb{E}_D[Err_{\text{out}}(g^{(D)}(x))] = \mathbb{E}_X\big[\mathbb{E}_D\big[(g^{(D)}(x) - \bar{g}(x))^2\big] + (\bar{g}(x) - f(x))^2\big].$$

Let's closely look at this formula. The errors are from two sources:

- **Variance**: $\mathbb{E}_D\big[(g^{(D)}(x) - \bar{g}(x))^2\big]$. Variance captures how much your classifier changes if you train on a different training set. We need to collect more data to reduce the variance.
- **Bias**: $(\bar{g}(x) - f(x))^2$. Bias is the inherent error that you obtain from your classifier even with infinite training data. We need to build a more complex model to reduce the bias.

However, if we reduce the bias, then the variance tends to increase.

5.1.1 Alternative Derivation

The derivation of the bias–variance decomposition for squared error proceeds as follows.[6][7] For notational convenience, abbreviate $f = f(x)$ and $\hat{f} = \hat{f}(x)$. First, recall that, by definition, for any random variable $\mathbf{X}$, we have

$$\operatorname{Var}\big[\hat{f}(x)\big] = \mathrm{E}[X^2] - \mathrm{E}[X]^2.$$

By rearranging, we get

$$\mathrm{E}[X^2] = \operatorname{Var}\big[\hat{f}(x)\big] + \mathrm{E}[X]^2.$$

Since f is deterministic

$$\mathrm{E}[f] = f$$

Thus, given $y = f + \varepsilon$ and $\mathrm{E}[\varepsilon] = 0$, implies $\mathrm{E}[y] = \mathrm{E}[f + \varepsilon] = \mathrm{E}[f] = f$

Also, since $\operatorname{Var}[\varepsilon] = \sigma^2$

$$\operatorname{Var}[y] = \mathrm{E}[(y - \mathrm{E}[y])^2] = \mathrm{E}[(y - f)^2] = \mathrm{E}[(f + \varepsilon - f)^2] = \mathrm{E}[\varepsilon^2] = \operatorname{Var}[\varepsilon] + \Big(\mathrm{E}[\varepsilon]\Big)^2 = \sigma^2$$

Thus, since ε and $\hat{f}$ are independent, we can write:

$$\begin{aligned}
\mathrm{E}\left[(y-\hat{f})^2\right] &= \mathrm{E}\left[(f+\varepsilon-\hat{f})^2\right] \\
&= \mathrm{E}\left[(f+\varepsilon-\hat{f}+\mathrm{E}[\hat{f}]-\mathrm{E}[\hat{f}])^2\right] \\
&= \mathrm{E}\left[(f-\mathrm{E}[\hat{f}])^2\right]+\mathrm{E}[\varepsilon^2]+\mathrm{E}\left[(\mathrm{E}[\hat{f}]-\hat{f})^2\right]+2\,\mathrm{E}\left[(f-\mathrm{E}[\hat{f}])\varepsilon\right]+ \\
&\quad 2\,\mathrm{E}\left[\varepsilon(\mathrm{E}[\hat{f}]-\hat{f})\right]+2\,\mathrm{E}\left[(\mathrm{E}[\hat{f}]-\hat{f})(f-\mathrm{E}[\hat{f}])\right] \\
&= (f-\mathrm{E}[\hat{f}])^2+\mathrm{E}[\varepsilon^2]+\mathrm{E}\left[(\mathrm{E}[\hat{f}]-\hat{f})^2\right]+ \\
&\quad 2(f-\mathrm{E}[\hat{f}])\,\mathrm{E}[\varepsilon]+2\,\mathrm{E}[\varepsilon]\,\mathrm{E}\left[\mathrm{E}[\hat{f}]-\hat{f}\right]+2\,\mathrm{E}\left[\mathrm{E}[\hat{f}]-\hat{f}\right](f-\mathrm{E}[\hat{f}]) \\
&= (f-\mathrm{E}[\hat{f}])^2+\mathrm{E}[\varepsilon^2]+\mathrm{E}\left[(\mathrm{E}[\hat{f}]-\hat{f})^2\right] \\
&= (f-\mathrm{E}[\hat{f}])^2+\mathrm{Var}[y]+\mathrm{Var}\left[\hat{f}\right] \\
&= \mathrm{Bias}[\hat{f}]^2+\mathrm{Var}[y]+\mathrm{Var}\left[\hat{f}\right] \\
&= \mathrm{Bias}[\hat{f}]^2+\sigma^2+\mathrm{Var}\left[\hat{f}\right]
\end{aligned}$$

Chapter 6

Optimization

6.1 Intuition of Gradient

Gradient descent is an optimization algorithm used to minimize a function by iteratively moving towards the function's minimum value. It is a fundamental concept in machine learning, particularly in training models such as neural networks. The gradient is a vector that represents the direction of the steepest increase of the function at a given point. For example, for a convex function $z = ax^2 + by^2$, the gradient is $[2ax, 2by]$, which points in the direction of the steepest ascent.

In gradient descent, the goal is to minimize the function, so the algorithm moves in the opposite direction of the gradient, which is $[-2ax, -2by]$. This opposite direction is chosen because it is the direction of the steepest decrease in the function value. But how do we know that moving in this direction will strictly decrease the function value?

6.1.1 Direction of Gradient Descent

Let's investigate the direction of gradient descent.

- The derivative of the objective function $f(\mathbf{x})$ provides the slope of $f(\mathbf{x})$ at the point $f(\mathbf{x})$.
- It tells us how to change $\mathbf{x}$ in order to make a small improvement in our goal.

A function $f(\mathbf{x})$ can be approximated by its first-order Taylor expansion at $\bar{\mathbf{x}}$:

$$f(\mathbf{x}) \approx f(\bar{\mathbf{x}}) + \nabla f(\bar{\mathbf{x}})^T (x - \bar{\mathbf{x}})$$

Now let $\mathbf{d} \neq 0, \|\mathbf{d}\| = 1$ be a direction, and in consideration of a new point $\mathbf{x} := \bar{\mathbf{x}} + \mathbf{d}$, we define:

$$f(\bar{\mathbf{x}} + \mathbf{d}) \approx f(\bar{\mathbf{x}}) + \nabla f(\bar{\mathbf{x}})^T \mathbf{d}$$

We would like to choose $\mathbf{d}$ that minimizes the function f. From the Cauchy-Schwarz inequality [1], we know that

$$|\nabla f(\bar{\mathbf{x}})^T \mathbf{d}| \leq \|\nabla f(\bar{\mathbf{x}})\| \, \|\mathbf{d}\|.$$

[1] Cauchy-Schwarz Inequaility: $|\mathbf{a} \cdot \mathbf{b}| \leq \|\mathbf{a}\| \, \|\mathbf{b}\|$. Equality holds if and only if either $\mathbf{a}$ or $\mathbf{b}$ is a multiple of the other.

The equality holds if and only if $\mathbf{d} = \lambda \nabla f(\bar{\mathbf{x}})$, where $\lambda \in \mathbb{R}$. Since we want to minimize the function f, we negate the steepest direction $\mathbf{d}^*$, then

$$f(\bar{\mathbf{x}} + \mathbf{d}) \approx f(\bar{\mathbf{x}}) - \lambda \nabla f(\bar{\mathbf{x}})^T \nabla f(\bar{\mathbf{x}}).$$

Since $\nabla f(\bar{\mathbf{x}})^T \nabla f(\bar{\mathbf{x}})$ is **always positive**, the term $-\lambda \nabla f(\bar{\mathbf{x}})^T \nabla f(\bar{\mathbf{x}})$ is always negative. Therefore by updating $\mathbf{x}$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \eta \nabla f(\mathbf{x}^{(k)}),$$

we get

$$f(\mathbf{x}^{(k+1)}) < f(\mathbf{x}^{(k)}).$$

6.2 Normalized Gradient Descent

The underlying issue of the vanila gradient descent is the presence of saddle points in nonconvex functions; the gradient $\nabla f(x)$ vanishes near saddle points, which causes GD to "stall" in neighboring regions. This both slows the overall convergence rate and makes detection of local minima difficult. The detrimental effects of this issue become particularly severe in high-dimensional problems where the number of saddle points may proliferate.

However, in the normalized gradient descent

$$\frac{\nabla f(x)}{\|\nabla f(x)\|}$$

The normalized gradient preserves the direction of the gradient but ignores magnitude, because the normalization does not vanish near saddle points, the intuitive expectation is that NGD should not slow down in the neighborhood of saddle points and should therefore escape quickly.

6.3 Projected Gradient Descent

Gradient Descent (GD) is a standard way to solve unconstrained optimization problem. Starting from an initial point $x \in \mathbb{R}^n$, GD itereates until a stopping criterion is met. Projected Gradient Descent (PGD) is a way to solve constrained optimization problem. Consider a constraint set $\mathcal{Q}$, starting from a initial point $x_0 \in \mathcal{Q}$, PGD iterates the following equation until a stopping condition is met:

$$x_{k+1} = P_{\mathcal{Q}}\Big(x_k - t_k \nabla f(x_k)\Big),$$

where $P_{\mathcal{Q}}$ is the projection operator

$$P_{\mathcal{Q}}(x_0) = \underset{x \in \mathcal{Q}}{\operatorname{argmin}} \frac{1}{2}\|x - x_0\|_2^2$$

In other words, given a point x_0, $P_{\mathcal{Q}}$ tries to to find a point $x \in \mathcal{Q}$ which is "closest"to x_0.

Note that a vector projection can be expressed as follows:

$$a_1 = \|\mathbf{a}\| \cos\theta = \mathbf{a} \cdot \hat{\mathbf{b}} = \mathbf{a} \cdot \frac{\mathbf{b}}{\|\mathbf{b}\|}$$

Thus, a projection for unit L_2 ball is given by the solution of the equation as follows:

$$\mathbf{x} = \mathcal{P}_{\|x\|_2 \leq 1}(\mathbf{y})$$

The solution is

$$\mathbf{x} = \frac{\mathbf{y}}{\max\{1, \|\mathbf{y}\|_2\}}$$

The "geometric" proof is given as follows: Let $\mathcal{S} = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_2 \leq 1\}$.

- If $\mathbf{y} \in \mathcal{S}$, then $\|y\|_2 \leq 1$ and $\mathbf{y}$ itself is the closest point to $\mathbf{y}$.
- If $\mathbf{y} \notin \mathcal{S}$, then $\|y\|_2 > 1$ and the closest point $\mathbf{x} \in \mathcal{S}$ to $\mathbf{y}$ will be simply $\frac{\mathbf{y}}{\|\mathbf{y}\|_2}$ as the norm of $\frac{\mathbf{y}}{\|\mathbf{y}\|_2} = 1$.

By combining the bost cases, we have

$$\mathbf{x} = \frac{\mathbf{y}}{\max\{1, \|\mathbf{y}\|_2\}}$$

6.4 Exponentially Weighted Average

$$v_t = \beta v_{t-1} + (1 - \beta)\theta_t$$

Larger β value covers more longer history. EMA is exponentially weighted average the previous result.

6.5 Bias Correction

The initial values of v_t will be very low which need to be compensated, since the curve starts from 0, there are not many values to average on in the initial points. Thus, the curve is lower than the correct value initially and then moves in line with expected values. The β is the same as the averaging coefficient. As t becomes large, the impact of the bias correction will be decreased.

$$v_t = \frac{v_t}{1 - \beta^t}$$

6.6 Momentum

Momentum can reduce the oscillation in the gradients. Let's say w has a small value and b is in charge of oscillation. Then momentum can cancel out db by averaging them.

$$\begin{aligned}
v_{dw} &= \beta v_{dw} + (1 - \beta)dw \\
v_{db} &= \beta v_{db} + (1 - \beta)db \\
w &= w - \alpha v_{dw} \\
b &= b - \alpha v_{db}
\end{aligned}$$

6.7 Adagrad: Adaptive Gradient

$$v_{dw} = v_{dw} + dw \cdot dw$$
$$w = w - \frac{\alpha}{\sqrt{v_{dw}} + \epsilon} v_{dw}$$

A con of Adagrad is learning rate will become very small

6.8 RMS Prop

$$s_{dw} = \beta s_{dw} + (1 - \beta) dw^2$$
$$s_{db} = \beta s_{db} + (1 - \beta) db^2$$
$$w = w - \alpha \frac{dw}{\sqrt{s_{dw}}}$$
$$b = b - \alpha \frac{db}{\sqrt{s_{db}}}$$

6.9 ADAM

Its name is derived from adaptive moment estimation, and the reason it's called that is because Adam uses estimations of first and second moments of gradient to adapt the learning rate for each weight of the neural network. N-th moment of a random variable is defined as the expected value of that variable to the power of n. More formally:

$$m_n = \mathbb{E}[X^n]$$

To estimates the moments, Adam utilizes exponentially moving averages, computed on the gradient evaluated on a current mini-batch:

Since m and v are estimates of first and second moments, we want to have the following property:

$$\mathbb{E}[m_t] = \mathbb{E}[g_t] \tag{6.1}$$
$$\mathbb{E}[v_t] = \mathbb{E}[g_t^2] \tag{6.2}$$

Unbiased estimators

ADAM uses both momentum style and RMS prop style averaging.

- $v_{dw} = \beta v_{dw} + (1 - \beta) dw$
- $v_{db} = \beta v_{db} + (1 - \beta) db$
- $s_{dw} = \beta s_{dw} + (1 - \beta) dw^2$

- $s_{db} = \beta s_{db} + (1 - \beta) db^2$

Using them,

- $v_{dw}^{\text{corr}} = \frac{v_{dw}}{1-\beta_1^t}$
- $v_{db}^{\text{corr}} = \frac{v_{db}}{1-\beta_1^t}$
- $s_{dw}^{\text{corr}} = \frac{s_{dw}}{1-\beta_2^t}$
- $s_{db}^{\text{corr}} = \frac{s_{db}}{1-\beta_2^t}$

Finally,

$$w = w - \alpha \frac{v_{dw}^{\text{corr}}}{\sqrt{s_{dw}^{\text{corr}}} + \varepsilon}$$
$$b = b - \alpha \frac{v_{db}^{\text{corr}}}{\sqrt{s_{db}^{\text{corr}}} + \varepsilon}$$

Chapter 7

Trees

A classification tree is a flowchart that helps a computer make decisions. It asks a series of yes/no questions about your data like "Is age ≤ 30"? and follows the answers down branches until it reaches a final box (a *leaf*). That leaf says which class the item belongs to, for example spam or not spam.

Trees are popular because they're easy to read and explain. You can show the rules to anyone on your team and they'll understand why a prediction was made. Trees also work well with mixed data (numbers and categories) and need very little data cleaning.

At each step, the tree tries many possible questions and picks the one that best separates the classes. We measure *how mixed* a node is using a number called *impurity* (common choices are *Gini* or *entropy*). A good question makes child nodes less mixed (ideally, each child is mostly one class).

Once a new example flows through the questions to a leaf, the tree predicts the majority class in that leaf. It can also report simple probabilities, like Class A: 80%, Class B: 20%, based on how the training examples in that leaf were labeled.

Deep trees can memorize the training data and make mistakes on new data (*overfitting*). You can control this by limiting the depth, requiring a minimum number of samples per split/leaf, or pruning back weak branches. When you need more accuracy and stability, ensembles like *Random Forests* or *Gradient Boosted Trees* build on the same idea but combine many trees.

Decision trees are more prone to overfitting than many of the models, as their learning algorithms can produce large, complicated decision trees that perfectly model every training instance but fail to generalize the real relationship. Several techniques can mitigate over-fitting in decision trees. *Pruning* is a common strategy that removes some of the tallest nodes and leaves of a decision tree.

7.1 Classification Tree

Let (p_k) be the fraction of samples of class (k) in the node. **Gini impurity**:

$$\text{Gini} = 1 - \sum_k p_k^2$$

- Range: $[0, 0.5]$ (0) (pure) to 0.5 ($p = 0.5$) for a binary class problem.

Entropy (information entropy)

$$H = -\sum_k p_k \log_2 p_k$$

- Range: (0) (pure) to ($\log_2 K$) (maximally mixed; for binary, max = 1 bit at ($p = 0.5$)).

In both cases, the node is pure when it has 0 impurity and maximally impure when classes are evenly mixed.

Example

A node with 80% class A, 20% class B: ($p = [0.8, 0.2]$)

- Gini: $1 - (0.8^2 + 0.2^2) = 1 - (0.64 + 0.04) = 0.32$
- Entropy: $-[0.8 \log_2 0.8 + 0.2 \log_2 0.2] \approx 0.72$ bits

A node with 60% / 40%: ($p = [0.6, 0.4]$)

- Gini: $1 - (0.36 + 0.16) = 0.48$
- Entropy ≈ 0.97 bits

How a split is scored (impurity decrease):

Trees choose the split that **reduces impurity** the most:

$$\text{Gain} = \text{Impurity(parent)} - \left(\tfrac{n_L}{n}\text{Impurity}(L) + \tfrac{n_R}{n}\text{Impurity}(R)\right)$$

Example

Let's say a node splits samples as follows:

- 100 samples, classes A/B = 60/40 (parent ($p = [0.6, 0.4]$))
- Candidate split: Left: 50 samples (40/10), Right: 50 samples (20/30)

The impurity of the node is given by

- Gini: 0.48,
- Entropy: ≈ 0.97

Then, we can compute the total Gini impurity, which is a weighted average of Gini impurities for the leaves,

- Left (40/10, ($p = [0.8, 0.2]$)):
  - Gini: 0.32,
  - Entropy: ≈ 0.72
- Right (20/30, ($p = [0.4, 0.6]$)):

  - Gini: 0.48
  - Entropy ≈ 0.97

Then,

- Gini: $0.5 \times 0.32 + 0.5 \times 0.48 = 0.40$.
  - Gain: $0.48 - 0.40 = 0.08$
- Entropy: $0.5 \times 0.72 + 0.5 \times 0.97 = 0.8465$
  - Gain $\approx 0.97 - 0.8465 = 0.1245$ bits

This split improves purity; you'd compare it with other candidate splits and pick the best gain.

Chapter 8

Ensemble Learning

8.1 Bagging

Bagging (bootstrap aggregating) is a simple way to make a noisy model more stable. Imagine you have a wobbly predictor-like a deep decision tree-that can change its mind a lot if the training data changes a little. Instead of trusting a single tree, bagging builds many versions of that model on slightly different views of the data, and then averages their answers (or takes a majority vote for classification). Averaging smooths out the noise, so the final prediction is steadier and usually more accurate.

How do we get those slightly different views? That's where bootstrapping comes in. From the original training set, we repeatedly draw new datasets of the same size with replacement (so the same example can appear multiple times, and some examples are left out). Each bootstrapped dataset trains its own model. Because each model sees a different sample, their mistakes won't line up perfectly—averaging then cancels out a lot of the randomness.

Why does this help? Many models, especially high-variance ones like decision trees, can overfit the quirks of a single dataset. Bagging reduces variance by blending many perspectives, without increasing bias too much. In practice, this often yields a solid accuracy boost and better reliability. A nice side effect is you get out-of-bag estimates: the examples left out of each bootstrap can be used as a built-in validation set to measure performance without a separate hold-out.

Bagging isn't magic—if the base model is already very stable (low variance) or consistently biased in the wrong direction, averaging won't fix the core problem. It also costs more compute and can feel less interpretable since you're dealing with many models instead of one. But as a foundational ensemble idea, bagging is both elegant and powerful—and it's the backbone of methods like Random Forests, which add an extra twist by randomly selecting features, too.

8.1.1 Intuition

We start with a single training set ($D = (x_i, y_i)_{i=1}^n$). Instead of hoping for many independent datasets, we **simulate** them by drawing **bootstrap samples** ($D_1, \ldots, D_M$): each (D_m) is formed by sampling (n) examples **with replacement** from (D). For each (D_m), we fit a base learner (h_m) (*e.g.,* a decision tree, ridge regression, logistic regression). We then **aggregate** the

models:

$$\bar{h}(x) = \frac{1}{M} \sum_{m=1}^{M} h_m(x).$$

If we could draw truly independent datasets $(D^{(1)}, \ldots, D^{(M)})$ from the population and train $(h^{D^{(m)}})$ on each, then the **empirical average hypothesis** would converge to the **theoretical average hypothesis** $(\mathbb{E}_D[h^D(x)])$ as $(M \to \infty)$. With bagging, our bootstraps come from the **empirical distribution** of (D), not the population, so they're not independent.

- Each bootstrap sample is just a reshuffled, reweighted version of the same original points.
- So two bootstrap samples will overlap a lot (they reuse the same observations), unlike two brand-new datasets collected from the real world.
- In short: they're new mixes of the same ingredients, not new ingredients.

Still, two facts make bagging effective:

1. **Variance reduction by averaging**: Training many models on these different mixes and averaging their predictions smooths out noise (reduces variance), especially for models that change a lot when the data changes (like deep trees).
2. **Bootstrap as a population proxy**: Drawing with replacement from (D) mimics sampling from the underlying data-generating process via the empirical distribution. This is not perfect independence, but for many learners it's good enough to bring $(\bar{h})$ close to $(\mathbb{E}_D[h^D(x)])$ in practice, especially for unstable learners (small data perturbations $\to$ large model changes), like deep decision trees.

8.1.2 Bias–variance intuition

- Variance: Bagging typically decreases variance because averaging stabilizes predictions.
- Bias: Bagging usually does not increase bias, and may slightly reduce it for some learners. But its main win is variance.
- Who benefits most? Unstable learners (*e.g.,* trees, k-NN with small (k)) benefit a lot. Stable learners (*e.g.,* linear/ridge regression) benefit less, though averaging can still help in noisy regimes.

Their are some costs:

- Interpretability
- Computational costs

When and why it works (and when it doesn't)

- Correlation matters. If base learners are too correlated, variance reduction is limited. This is why Random Forests add feature subsampling at each split to further decorrelate trees, improving over plain bagging of trees.
- Computational cost. Training (M) models costs $(M\times)$ as much compute (though it parallelizes nicely).
- Interpretability. An averaged ensemble is harder to interpret than a single model (especially vs. a small tree or linear model). You can mitigate with feature importance, partial dependence, SHAP, and so on., but it's still less transparent.
- Diminishing returns in (M). Gains flatten as (M) grows because you approach the correlation floor. In practice, tens to a few hundreds of models are often sufficient.

8.2 Boosting

Boosting builds a strong model by adding many small, simple models (weak learners) sequentially. Each new model focuses on the mistakes of the models before it. In the end, we add their predictions to get one strong predictor.

- Bagging = parallel averaging to reduce **variance**.
- Boosting = sequential fixing to reduce **bias** (and often variance too).

Types of Boosting Algorithms:

- AdaBoost (Adaptive Boosting)
- Gradient Boosting
- XGBoost

8.3 AdaBoost

Boosting is a general strategy for learning classifiers by combining simpler ones. The idea of boosting is to take a "weak classifier" - that is, any classifier that will do at least slightly better than chance — and use it to build a much better classifier, thereby boosting the performance of the weak classification algorithm. This boosting is done by averaging the outputs of a collection of weak classifiers.

The most popular boosting algorithm is *AdaBoost*, so-called because it is "adaptive." AdaBoost is extremely simple to use and implement (far simpler than SVMs), and often gives very effective results. There is tremendous flexibility in the choice of weak classifier as well. Boosting is a specific example of a general class of learning algorithms called ensemble methods, which attempt to build better learning algorithms by combining multiple simpler algorithms.

Suppose we are given training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$, where $\mathbf{x}_i \in \mathbb{R}^K$ and $y_i \in \{-1, 1\}$. And suppose we are given a (potentially large) number of weak classifiers, denoted $f_m(\mathbf{x}) \in \{-1, 1\}$, and a **0-1**

loss function I, defined as

$$I(f_m(\mathbf{x}), y) = \begin{cases} 0 & \text{if } f_m(\mathbf{x}_i) = y_i \\ 1 & \text{if } f_m(\mathbf{x}_i) \neq y_i \end{cases}$$

- $I = 0$ if prediction equals the truth ($\hat{y} = y$)
- $I = 1$ if prediction is wrong ($\hat{y} \neq y$)

AdaBoost aims to build a strong classifier by combining many weak ones. It does this in rounds $m = 1, 2, \ldots, M$:

1. Give every training example the same weight. Every sample is equally important at the beginning.
2. Fit a *weak learner* f_m on the weighted data
3. Compute how good it is: measure its *weighted error* of weak learner, e_m.

   $$e_m = \sum_{i=1}^{N} w_i^m \cdot I(f_m(\mathbf{x}_i), y_i),$$

   where w_i^m is the current example weight.

   - This measures how many (weighted) mistakes that stump/tree makes this round.
4. Compute α_m, which is the *vote weight* (strength) assigned to that weak learner when forming the final ensemble:

   $$\alpha_m = \frac{1}{2} \ln \left(\frac{1 - e_m}{e_m} \right).$$

   - minimizing the weighted exponential loss for fixed f_m.
   - bigger when the error e_m is smaller
   - As $e_m \to 0$, $\alpha_m \to \infty$.
   - As $e_m \to 1$, $\alpha_m \to -\infty$.
5. Repeat: fit the next weak learner on the reweighted data, and so on.

   $$w_i^{(m+1)} \propto w_i^{(m)} \cdot \exp(-\alpha_m y_i f_m(\mathbf{x}_i)).$$

After learning, the final classifier is based on a linear combination of the weak classifiers:

$$F(\mathbf{x}) = \sum_{m=1}^{M} \alpha_m f_m(\mathbf{x}).$$

If more of the strong (high-α) weak learners say $+1$ than -1, the final answer is $+1$, etc.

This is why it's called **adaptive:** each new weak learner adapts to the mistakes of the previous ones by focusing more weight on hard examples.

8.4 Gradient Boosting

Part II

Regression

Chapter 9

Introduction to Regression Methods

9.1 Introduction

Regression is a process for finding the relationship between the inputs and the outputs. In a regression problem, we consider a set of noisy measurement (or noisy output data) $\mathbf{y} = [y_1, \ldots, y_d]^T$ with measurement noise $\boldsymbol{\eta} = [\eta_1, \ldots, \eta_d]^T$. We also consider a set of input data $\mathbf{x} = [x_1, \ldots, x_d]$. We call the set of these input-output pairs $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_m, \mathbf{y}_m)\}$ the training data. The true relationship between the input and the output data is unknown. We denote this unknown relationship as a mapping $f(\cdot)$ that takes $\mathbf{x}_n$ and maps it to y_n,

$$\mathbf{y} = f(\mathbf{x}).$$

Finding the true $f(\cdot)$ from a finite number of data points D is infeasible. There are infinitely many ways to design $f(\cdot)$ for every $\mathbf{x}_i$. The idea of regression is to add a structure to the problem. Instead of looking for the true $f(\cdot)$, we find a proxy $g_\theta(\cdot)$ that takes a certain parameters $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_d]^T$. For instance, we can postulate that $(\mathbf{x}_n, \mathbf{y}_n)$ has a linear relationship:

$$g_{\boldsymbol{\theta}}(\mathbf{y}) = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\eta},$$

where $\mathbf{X}$ is a $m \times d$ input matrix (or our observations). Since we do not know the true relationship, any choice of model is our conjecture. However, we can model the error of our choice. Given a parameter $\boldsymbol{\theta}$, we consider the difference between the noisy measurements and estimated value as follows:

$$\boldsymbol{\epsilon} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}$$

The purpose of regression is to find the best $\boldsymbol{\theta}$ such that the error is minimized. Therefore, we can consider a following objective function:

$$J(\boldsymbol{\theta}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon}$$

Note that this is equivalent to minimizing the mean squared error:

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \mathbf{x}_i \boldsymbol{\theta})^2.$$

We can optimize this in a closed-form as follows:

$$\begin{aligned} J(\boldsymbol{\theta}) &= \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ &= (\mathbf{y}^T - \boldsymbol{\theta}^T \mathbf{X}^T)(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ &= \mathbf{y}^T \mathbf{y} - \boldsymbol{\theta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\theta} \end{aligned}$$

To find the $\boldsymbol{\theta}$ that minimizes the objective function, we will compute a derivative of the function while setting it equal to zero:

$$\begin{aligned}\frac{\partial J}{\partial \boldsymbol{\theta}} &= -\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta} = 0 \\ &\Rightarrow \mathbf{X}^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y}) = 0 \\ \boldsymbol{\theta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

Note that the $\mathbf{X}^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$ is called the *normal equation*.

```python
import numpy as np
import matplotlib.pyplot as plt

N = 50
x = np.random.randn(N)
w_1 = 3.4 # True Parameter
w_0 = 0.9 # True Parameter
y = w_1*x + w_0 + 0.3*np.random.randn(N) # Synthesize training data

X = np.column_stack((x, np.ones(N)))
W = np.array([w_1, w_0])

# From Scratch
XtX    = np.dot(X.T, X)
XtXinvX = np.dot(np.linalg.inv(XtX), X.T) # d x m
W_best = np.dot(XtXinvX, y.T)
print(f"W_best: {W_best}")

# Pythonic Approach
theta = np.linalg.lstsq(X, y, rcond=None)[0]
print(f"Theta: {theta}")

t = np.linspace(0, 1, 200)
y_pred = W_best[0]*t+W_best[1]
yhat = theta[0]*t+theta[1]
plt.plot(x, y, 'o')
plt.plot(t, y_pred, 'r', linewidth=4)
plt.show()
```

9.1.1 MLE Interpretation

If we assume $\boldsymbol{\epsilon}_i \sim \mathcal{N}(0, \sigma^2)$, then

$$y_i|\mathbf{x}_i \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2).$$

Thus, the likelihood (*i.e.,* the probability density of the observations given the parameters) function is given by

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = p(\mathbf{y}|X, \boldsymbol{\theta}) = \prod_i^n p(y_i|\mathbf{x}_i, \boldsymbol{\theta}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \boldsymbol{\theta}\mathbf{x}_i)^2}{2\sigma^2}\right)$$

$$\log \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = \text{const} - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - \boldsymbol{\theta}\mathbf{x}_i)^2$$

For a fixed σ, it is equivalent to minimizing the MSE.

9.1.2 Time Complexity

The time complexity of the training process involves the following steps:

- Computing $X^T X$: The product $X^T X$ involves multiplying a $d \times m$ matrix with an $m \times d$ matrix. The time complexity of this matrix multiplication is $O(md^2)$.
- Computing $X^T \mathbf{y}$: $X^T \mathbf{y}$ involves multiplying a $d \times m$ matrix with an $m \times 1$ vector. - The time complexity is $O(md)$.
- Computing $\left(X^T X\right)^{-1}$: - The inversion of a $d \times d$ matrix $X^T X$ has a time complexity of $O(d^3)$.
- Multiplying $\left(X^T X\right)^{-1}$ with $X^T \mathbf{y}$: This is a matrix-vector multiplication involving a $d \times d$ matrix and a $d \times 1$ vector. Thus, the time complexity is $O(d^2)$.
- Total Training Time Complexity: The dominant terms in the training process are $O(md^2)$ (for computing $X^\top X$) and $O(d^3)$ (for inverting $X^T X$). - Therefore, the total time complexity for training a linear regression model is $O(md^2 + d^3)$.

Inference time complexity:

- The inference step requires a matrix-vector multiplication between an $m' \times d$ inference data matrix and a $d \times 1$ vector. - The time complexity of this operation is $O(m'd)$.

9.2 Overdetermined and Underdetermined Systems

Recall that the linear regression problem is an optimization problem of finding the optimal parameter as follows:

$$\boldsymbol{\theta}_{opt} = \underset{\boldsymbol{\theta} \in \mathbb{R}^d}{\operatorname{argmin}} ||y - \mathbf{X}\boldsymbol{\theta}||^2.$$

We say the optimization problem is *overdetermined* if $\mathbf{X} \in \mathbb{R}^{m \times d}$ is tall and skinny, *i.e.,* $m > d$. This problem has a unique solution $\boldsymbol{\theta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ if and only if $\mathbf{X}^T \mathbf{X}$ is invertible. Equivalently, $\mathbf{X}$ should be linearly independent (*i.e.,* full rank).

If $\mathbf{X}$ is fat and short (*i.e.,* $m < d$), a problem is called *underdetermined*. **This problem will have infinitely many solutions**. Among all the feasible solutions, we will pick the one that minimizes the squared norm. The solution is called the *minimum-norm* least squares. Consider an underdetermined linear regression problem:

$$\boldsymbol{\theta} = \underset{\boldsymbol{\theta} \in \mathbb{R}^d}{\operatorname{argmin}} \|\boldsymbol{\theta}\|^2, \text{ subject to } \mathbf{y} = \mathbf{X}\boldsymbol{\theta},$$

where $\mathbf{X} \in \mathbb{R}^{m \times d}, \boldsymbol{\theta} \in \mathbb{R}^d$, and $\mathbf{y} \in \mathbb{R}^m$. If the matrix has $\operatorname{rank}(\mathbf{X}) = m$, then the linear regression problem will have a unique global minimum

$$\boldsymbol{\theta} = \mathbf{X}^T (\mathbf{X}\mathbf{X}^T)^{-1} \mathbf{y}.$$

This solution is called the minimum-norm least-squares solution. The proof of this solution is given by:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\lambda}) = \|\boldsymbol{\theta}\|^2 + \boldsymbol{\lambda}^T (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}),$$

where $\boldsymbol{\lambda}$ is a Lagrange multiplier. The solution of the constrained optimization is the stationary point of the Lagrangian. To find it, we take the derivatives w.r.t., $\boldsymbol{\lambda}$ and $\boldsymbol{\theta}$ as follows:

$$\nabla_{\boldsymbol{\theta}} = 2\boldsymbol{\theta} + \mathbf{X}^T\boldsymbol{\lambda} = 0$$
$$\nabla_{\boldsymbol{\lambda}} = \mathbf{X}\boldsymbol{\theta} - \mathbf{y} = 0$$

The first equation gives us $\boldsymbol{\theta} = -\mathbf{X}^T\boldsymbol{\lambda}/2$. Substituting it into the second equation, and assuming that $\text{rank}(\mathbf{X}) = m$ so that $\mathbf{X}^T\mathbf{X}$ is invertible, we have $\boldsymbol{\lambda} = -2(\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{y}$. Thus, we have

$$\boldsymbol{\theta} = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{y}.$$

Note that $\mathbf{X}\mathbf{X}^T$ is often called a *Gram matrix*, $\mathbf{G}$.

9.3 Overfitting

We examine the relationship between the number of training samples and the complexity of the model.

9.4 Ridge Regression

Regularization means that instead of seeking the model parameters by minimizing the training loss alone, we add a penalty term to force the parameters to "behave better".

With the ridge regression principle, we can optimize it as follows:

$$\begin{aligned}
J(\boldsymbol{\theta}) &= \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda\|\boldsymbol{\theta}\|_2^2 && (9.1)\\
&= (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta} && (9.2)\\
&= (\mathbf{y}^T - \boldsymbol{\theta}^T\mathbf{X}^T)(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta} && (9.3)\\
&= \mathbf{y}^T\mathbf{y} - \boldsymbol{\theta}^T\mathbf{X}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T\lambda\mathbf{I}\boldsymbol{\theta} && (9.4)\\
\frac{\partial J}{\partial \boldsymbol{\theta}} &= -\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{y} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + 2\lambda\mathbf{I}\boldsymbol{\theta} = 0 && (9.5)\\
\boldsymbol{\theta} &= (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} && (9.6)
\end{aligned}$$

- If $\lambda \to 0$, then $\|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \underbrace{\lambda\|\boldsymbol{\theta}\|_2^2}_{=0}$
- $\lambda \to \infty$, then $\underbrace{\frac{1}{\lambda}\|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2}_{=0} + \|\boldsymbol{\theta}\|_2^2$, since what we want to do is to minimize the objective function, we can divide it by λ. Therefore, the solution will be $\boldsymbol{\theta} = 0$, because it is the smallest value the squared function can achieve.

Note that $\mathbf{X}^T\mathbf{X}$ is always symmetric [1]. Thus, it can be decomposed as $Q\Lambda Q^T$ by the Spectral theorem. The Q and Λ are eigenvector and eigenvalue matrices, respectively. Then, the inverse

[1] $(\mathbf{X}^T\mathbf{X})^T = \mathbf{X}^T\mathbf{X}$.

operation in the ridge regression can be expressed as follows:

$$\begin{aligned}\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} &= \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T + \lambda\mathbf{I} \\ &= \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T + \lambda\mathbf{Q}\mathbf{Q}^T \\ &= \mathbf{Q}(\mathbf{\Lambda} + \lambda\mathbf{I})\mathbf{Q}^T.\end{aligned}$$

Even if the symmetric matrix is not invertible or close to not invertible, the regularization constant λ makes it invertible (by making it to be a full-rank).

Note that we can change the ridge regression into a dual form:

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} \tag{9.7}$$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = \mathbf{X}^T\mathbf{y} \tag{9.8}$$

$$\boldsymbol{\theta} = \lambda^{-1}\mathbf{I}(\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\boldsymbol{\theta}) \tag{9.9}$$

$$= \mathbf{X}^T\underbrace{\lambda^{-1}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})}_{=\alpha} \tag{9.10}$$

$$= \mathbf{X}^T\alpha \tag{9.11}$$

This tells us that $\boldsymbol{\theta}$ is a linear combination of $\boldsymbol{X}$ (*i.e.,* training data points) with α. Then,

$$\lambda\alpha = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \tag{9.12}$$

$$= (\mathbf{y} - \mathbf{X}\mathbf{X}^T\alpha) \tag{9.13}$$

$$\mathbf{y} = (\mathbf{X}\mathbf{X}^T\alpha + \lambda\alpha) \tag{9.14}$$

$$\alpha = (\mathbf{X}\mathbf{X}^T + \lambda)^{-1}\mathbf{y} \tag{9.15}$$

$$= (\mathbf{G} + \lambda)^{-1}\mathbf{y}. \tag{9.16}$$

This gives us the solution of the *underdetermined* problems. For a new data point $\mathbf{x}_{new}$, we can make an inference by computing dot products between the new data point and each training data point:

$$\begin{aligned}y &= \boldsymbol{\theta}^T\mathbf{x}_{new} \\ &= \alpha^T\mathbf{X}\mathbf{x}_{new}\end{aligned}$$

9.4.1 Time Complexity

- Training time: $O(md^2 + m^3)$
- Inference time: $O(md)$

9.5 Weighted LSE

The OLEs assume an equal confidence on all the measurements. Now we look at varying confidence in the measurements. We assume that the noise for each measurement has zero mean and is independent, then the covariance matrix for all measurement noise is given by

$$\begin{aligned}R &= \mathbb{E}(\eta\eta^T) \\ &= \begin{bmatrix}\sigma_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_l^2\end{bmatrix}\end{aligned}$$

By denoting the error vector $\mathbf{y} - \mathbf{X}\boldsymbol{\theta}$ as $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_l)^T$, we will minimize the sum of squared differences weighted over the variations of the measurements:

$$\begin{aligned} J(\tilde{\mathbf{x}}) = \boldsymbol{\epsilon}^T R^{-1} \boldsymbol{\epsilon} &= \frac{\boldsymbol{\epsilon}_1^2}{\sigma_1^2} + \cdots + \frac{\boldsymbol{\epsilon}_l^2}{\sigma_l^2} \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T R^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \end{aligned}$$

Note that by dividing each residual by its variance, we effectively equalize the influence of each data point on the overall fitting process. Subsequently, by taking the partial derivative of J with respect to $\boldsymbol{\theta}$, we get the best estimate of the parameter, which is given by

$$\boldsymbol{\theta} = (\mathbf{X}^T R^{-1} \mathbf{X})^{-1} \mathbf{X}^T R^{-1} \mathbf{y}.$$

Note that the measurement noise matrix R must be non-singular for a solution to exist.

9.6 Robust Linear Regression

The linear regression is based on the squared error criterion. This criterion often suffers from a serious drawback caused by outliers. By the definition of a squared error, our training loss is given by

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{n=1}^{N} \Big(y_n - g_{\boldsymbol{\theta}}(x_n) \Big)^2.$$

Let's assume that one of these error terms is large due to an outlier.

$$\mathcal{L}(\boldsymbol{\theta}) = \Big(y_1 - g_{\boldsymbol{\theta}}(x_1) \Big)^2 + \underbrace{\Big(y_2 - g_{\boldsymbol{\theta}}(x_2) \Big)^2}_{\text{Large}} + \cdots$$

If one or a few of these individual error terms are large, the square operation will amplify them. Consequently, the outliers suddenly have a very large contribution to the error. Since the goal of linear regression is to minimize the total loss, the presence of the outliers will drive the optimization solution to compensate for the large error.

Chapter 10

Recursive Least Squares

10.1 Recursive Least Squares

The ordinary least-squares assumes that all measurements are available at a certain time. However, this often might not be the case in practice. **More often, we obtain measurements sequentially and want to update our estimate with each new measurement.** In this case, the matrix $\mathbf{X}$ needs to be augmented. This update can be very expensive especially if the number of measurements is extremely large, the solutions of the least squares problem become prohibitive to compute.

This motivates the Recursive Least Squares (RLS). Suppose we have an estimate $\boldsymbol{\theta}_{k-1}$ after $(k-1)$ measurements and obtain a new measurement $\mathbf{y}_k$. How can we update our estimate without completely reworking on the pseudo-inverse problem?

A linear recursive estimator can be expressed in the following form:

$$\begin{aligned}\mathbf{y}_k &= \mathbf{X}_k\boldsymbol{\theta} + \boldsymbol{\eta}_k \\ \boldsymbol{\theta}_k &= \boldsymbol{\theta}_{k-1} + K_k(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1})\end{aligned}$$

Here, $\mathbf{X}_k$ is an $m \times d$ matrix (observations) and K_k is $d \times m$ and referred to as the *estimator gain matrix*. We refer to $(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1})$ as the *correction term*. Also, $\boldsymbol{\eta}_k$ is the measurement error. The new estimate is modified from the previous estimate $\boldsymbol{\theta}_{k-1}$ with a correction via the gain matrix.

Intuitively, we can notice that we have to compute the optimal gain matrix to update our estimate. To this end, we have to set an *estimation error*, which is our learning objective. The error can be expressed as follows:

$$\begin{aligned}\boldsymbol{\epsilon}_k &= \boldsymbol{\theta} - \boldsymbol{\theta}_k \\ &= \boldsymbol{\theta} - \boldsymbol{\theta}_{k-1} - K_k(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1}) \\ &= \boldsymbol{\epsilon}_{k-1} - K_k(\mathbf{X}_k\boldsymbol{\theta} + \boldsymbol{\eta}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1}) \\ &= \boldsymbol{\epsilon}_{k-1} - K_k\mathbf{X}_k(\boldsymbol{\theta} - \boldsymbol{\theta}_{k-1}) - K_k\boldsymbol{\eta}_k \\ &= (I - K_k\mathbf{X}_k)\boldsymbol{\epsilon}_{k-1} - K_k\boldsymbol{\eta}_k,\end{aligned}$$

where I is the $d \times d$ identity matrix. The mean of this error is then

$$\mathbb{E}[\boldsymbol{\epsilon}_k] = (I - K_k\mathbf{X}_k)\mathbb{E}[\boldsymbol{\epsilon}_{k-1}] - K_k\mathbb{E}[\boldsymbol{\eta}_k]$$

If $\mathbb{E}[\boldsymbol{\eta}_k] = 0$ and $\mathbb{E}[\boldsymbol{\epsilon}_{k-1}] = 0$, then $\mathbb{E}[\boldsymbol{\epsilon}_k] = 0$. So if the measurement noise has zero mean for all k, and the initial estimate of $\boldsymbol{\theta}$ is set equal to its expected value, then $\boldsymbol{\theta}_k = \boldsymbol{\theta}_k, \forall k$. This property tells us that the estimator $\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + K_k(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1})$ is *unbiased*. This property holds regardless of the value of the gain vector K_k. This means the estimate will be equal to the true value $\boldsymbol{\theta}$ on average.

The key is to **determine the optimal value of the gain vector** K_k. The optimality criterion is to **minimize the aggregated variance of the estimation errors at time** k:

$$\begin{aligned} J_k &= \mathbb{E}[\|\boldsymbol{\theta} - \boldsymbol{\theta}_k\|^2] \\ &= \mathbb{E}[\boldsymbol{\epsilon}_k^T \boldsymbol{\epsilon}_k] \\ &= \mathbb{E}[tr(\boldsymbol{\epsilon}_k \boldsymbol{\epsilon}_k^T)] \\ &= tr(P_k), \end{aligned}$$

where $P_k = \mathbb{E}[\boldsymbol{\epsilon}_k \boldsymbol{\epsilon}_k^T]$ is *the estimation-error covariance* (*i.e.,* **covariance matrix**). Note that the third line holds by the trace of a product (*i.e., cyclic property*) and the expectation in the third line can go into the trace operator by its linearity. Next, we can obtain P_k by

$$P_k = \mathbb{E}\Big[\big((I - K_k\mathbf{X}_k)\boldsymbol{\epsilon}_{k-1} - K_k\boldsymbol{\eta}_k\big)\big((I - K_k\mathbf{X}_k)\boldsymbol{\epsilon}_{k-1} - K_k\boldsymbol{\eta}_k\big)^T\Big]$$

By rearranging the above equation with the property that the mean of noise is zero, we can get

$$P_k = (I - K_k\mathbf{X}_k)P_{k-1}(I - K_k\mathbf{X}_k)^T + K_k R_k K_k^T, \tag{10.1}$$

where $R_k = \mathbb{E}[\boldsymbol{\eta}_k \boldsymbol{\eta}_k^T]$ as covariance of $\boldsymbol{\eta}_k$. This equation is the recurrence for the covariance of the least squares estimation error. It is consistent with the intuition that as the measurement noise R_k increases, the uncertainty in our estimate also increases (*i.e.,* P_k increases). Note that P_k should be positive definite since it is a covariance matrix.

Next, let's compute K_k that minimizes the cost function given by the error equation. We are going to utilize the following property:

$$\begin{aligned} \frac{\partial tr(CA^T)}{\partial A} &= C \\ \frac{\partial tr(ACA^T)}{\partial A} &= AC + AC^T \end{aligned}$$

Next, we are going to take a derivative to the objective function:

$$\begin{aligned} \frac{\partial J_k}{\partial K_k} = \frac{\partial tr(P_k)}{\partial K_k} &= \frac{\partial tr}{\partial K_k}\underbrace{(I - K_k\mathbf{X}_k)P_{k-1}(I - K_k\mathbf{X}_k)^T}_{=ACA^T} + \frac{\partial}{\partial K_k}tr\left(K_k R_k K_k^T\right) \\ &= \frac{\partial tr(ACA^T)}{\partial(I - K_k\mathbf{X}_k)}\frac{\partial(I - K_k\mathbf{X}_k)}{\partial K_k} + \frac{\partial}{\partial K_k}tr\left(K_k R_k K_k^T\right) \quad \text{by Chain Rule} \\ &= \left((I - K_k\mathbf{X}_k)P_{k-1} + (I - K_k\mathbf{X}_k)P_{k-1}^T\right)(-\mathbf{X}_k^T) + \frac{\partial}{\partial K_k}tr\left(K_k R_k K_k^T\right) \\ &= 2(I - K_k\mathbf{X}_k)P_{k-1}(-\mathbf{X}_k^T) + \frac{\partial}{\partial K_k}tr\left(K_k R_k K_k^T\right) \quad \text{, since } P_{k-1} \text{ is symmetric.} \\ &= -2(I - K_k\mathbf{X}_k)P_{k-1}\mathbf{X}_k^T + 2K_k R_k \end{aligned}$$

By setting the partial derivative to zero, we get

$$K_k = P_{k-1}\mathbf{X}_k^T(\mathbf{X}_k P_{k-1}\mathbf{X}_k^T + R_k)^{-1}.$$

10.1.1 Alternative Form

Sometimes it is useful to write the equations for P_k and K_k in alternate forms. Although these alternate forms are mathematically identical, they can be beneficial from a computational point of view. Let's first set $\mathbf{X}_k P_{k-1} \mathbf{X}_k^T + R_k = S_k$, then we get

$$K_k = P_{k-1} \mathbf{X}_k^T S_k^{-1}.$$

By putting this into Eq. (10.1),

$$\begin{aligned} P_k &= (I - P_{k-1}\mathbf{X}_k^T S_k^{-1}\mathbf{X}_k) P_{k-1} (I - P_{k-1}\mathbf{X}_k^T S_k^{-1}\mathbf{X}_k)^T + P_{k-1}\mathbf{X}_k^T S_k^{-1} R_k S_k^{-1} \mathbf{X}_k P_{k-1} \\ &\vdots \\ &= P_{k-1} - P_{k-1}\mathbf{X}_k^T S_k^{-1} \mathbf{X}_k^T P_{k-1} \\ &= (I - K_k \mathbf{X}_k) P_{k-1}. \end{aligned}$$

Note that P_k is symmetric (*c.f.*, $P_k = \boldsymbol{\epsilon}_k \boldsymbol{\epsilon}_k^T$), since it is a covariance matrix, and so is S_k.

We take the inverse of both sides of

$$P_{k-1}^{-1} = \left(\underbrace{P_{k-1}}_{A} - \underbrace{P_{k-1}\mathbf{X}_k^T}_{B} \big(\underbrace{\mathbf{X}_k P_{k-1} \mathbf{X}_k^T}_{D} \big)^{-1} \underbrace{\mathbf{X}_k P_{k-1}}_{C} \right)^{-1}.$$

Next, we apply the matrix inversion lemma which is known as *Sherman-Morrison-Woodbury matrix identity* (or *matrix inversion lemma*) identity:

$$(A - BD^{-1}C)^{-1} = A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1}.$$

Then, rewrite P_k^{-1} as follows:

$$\begin{aligned} P_k^{-1} &= P_{k-1}^{-1} + P_{k-1}^{-1} P_{k-1} \mathbf{X}_k^T \big((\mathbf{X}_k P_{k-1} \mathbf{X}_k^T + R_k) - \mathbf{X}_k P_{k-1} P_{k-1}^{-1} (P_{k-1} \mathbf{X}_k^T) \big)^{-1} \mathbf{X}_k P_{k-1} P_{k-1}^{-1} \\ &= P_{k-1}^{-1} + \mathbf{X}_k^T R_k^{-1} \mathbf{X}_k \end{aligned}$$

This yields an alternative expression for the covariance matrix:

$$P_k = \left(P_{k-1}^{-1} + \mathbf{X}_k^T R_k^{-1} \mathbf{X}_k \right)^{-1}$$

We can also obtain

$$K_k = P_k \mathbf{X}_k^T R_k^{-1}$$

By

$$\begin{aligned} P_k &= (I - K_k \mathbf{X}_k) P_{k-1} \\ P_k P_{k-1}^{-1} &= (I - K_k \mathbf{X}_k) \\ P_k P_k^{-1} &= P_k P_{k-1}^{-1} + P_k \mathbf{X}_k^T R_k^{-1} \mathbf{X}_k = I \\ I &= (I - K_k \mathbf{X}_k) + P_k \mathbf{X}_k^T R_k^{-1} \mathbf{X}_k \\ K_k &= P_k \mathbf{X}_k^T R_k^{-1}. \end{aligned}$$

10.1.2 Summary of RLS

In sum, RLS can be updated as follows:

- Update the gain matrix:
  - $K_k = P_{k-1}\mathbf{X}_k^T(\mathbf{X}_k P_{k-1}\mathbf{X}_k^T + R_k)^{-1}$ or
  - $K_k = P_k \mathbf{X}_k^T R_k^{-1}$
- Update estimate: $\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + K_k(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1})$
- Update error covariance matrix by either:
  - $P_k = (I - K_k\mathbf{X}_k)P_{k-1}$.
  - $P_k = (I - K_k\mathbf{X}_k)P_{k-1}(I - K_k\mathbf{X}_k)^T + K_k R_k K_k^T$,

Example: At sample time k, our measurement is

- $y_k = X_k\theta + \eta_k$
- $X_k = 1$
- $R_k = \mathbb{E}[\eta_k^2]$

For this scalar problem, the measurement matrix X_k is a scalar too, and the measurement noise covariance R_k is also a scalar. We will suppose that each measurement has the same covariance so the measurement covariance R_k is not a function of k, and can be written as R. Initially, before we have any measurements, we have some idea about the value of the θ, and this forms our initial estimate. We also have some uncertainty about our initial estimate, and this forms our initial covariance:

$$\begin{aligned}\hat{\theta}_0 &= \mathbb{E}[\theta] \\ P_0 &= \mathbb{E}[(\theta - \hat{\theta}_0)(\theta - \hat{\theta}_0)^T] \\ &= \mathbb{E}[(\theta - \hat{\theta}_0)^2]\end{aligned}$$

If we have absolutely no idea about θ, then $P(0) = \infty I$. If we are 100% certain about the θ before taking any measurements, then $P(0) = 0$. Let's compute the gain matrix at $k = 1$ by using the following equation:

$$K_k = P_{k-1}\mathbf{X}_k^T(\mathbf{X}_k P_{k-1}\mathbf{X}_k^T + R_k)^{-1}.$$

Then, we get

$$K_1 = P_0(P_0 + R)^{-1}.$$

Similarly, by

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + K_k(\mathbf{y}_k - \mathbf{X}_k\boldsymbol{\theta}_{k-1}),$$

we obtain

$$\hat{\theta}_1 = \hat{\theta}_0 + \frac{P_0}{P_0 + R}(y_1 - \hat{\theta}_0).$$

Finally, let's update our covariance matrix P_k by

$$P_k = (I - K_k \mathbf{X}_k) P_{k-1} (I - K_k \mathbf{X}_k)^T + K_k R_k K_k^T.$$

Then,

$$\begin{aligned} P_1 &= \left(I - \frac{P_0}{P_0 + R} \right) P_0 I - \frac{P_0}{P_0 + R} + \frac{P_0}{P_0 + R} R \frac{P_0}{P_0 + R} \\ &= \left(\frac{P_0 R^2}{(P_0 + R)^2} \right) + \frac{P_0^2 R}{(P_0 + R)^2} \\ &= \frac{P_0 R (P_0 + R)}{(P_0 + R)^2} \\ &= \frac{P_0 R}{P_0 + R} \end{aligned}$$

By repeating these calculations, we can update the above parameters and find general expressions:

$$\begin{aligned} P_{k-1} &= \frac{P_0 R}{(k-1) P_0 + R} \\ K_k &= \frac{P_0}{k P_0 + R} \\ \hat{\theta}_k &= \frac{(k-1) P_0 + R}{k P_0 + R} \hat{\theta}_{k-1} + \frac{P_0}{k P_0 + R} y_k \end{aligned}$$

Note that if θ is known perfectly *a priori* (*i.e.,* θ is known perfectly before any measurements are obtained) then $P_0 = 0$ and the above equation show that $K_k = 0$ and $\hat{\theta} = \hat{\theta}_0$. That is, the optimal estimate of θ is independent of any measurements that are obtained. In sum, this indicates that no update from measurements is needed, as the estimate is already perfect.

On the other hand, if x is completely unknown a priori, then $P_0 \to \infty$, and the above equations simplify to

$$\begin{aligned} \hat{\theta}_k &= \frac{(k-1) P_0}{k P_0} \hat{\theta}_{k-1} + \frac{P_0}{k P_0} y_k \\ &= \frac{k-1}{k} \hat{\theta}_{k-1} + \frac{1}{k} y_k \\ &= \frac{1}{k} [(k-1) \hat{\theta}_{k-1} + y_k] \end{aligned}$$

In other words, the optimal estimate of θ is equal to the running average of the measurements y_k, which can be written as

$$\begin{aligned} \bar{y}_k &= \frac{1}{k} \sum_{j=1}^{k} y_j \\ &= \frac{1}{k} \left(\sum_{j=1}^{k-1} y_j + y_k \right) \\ &= \frac{1}{k} \left[(k-1) \frac{1}{k-1} \sum_{j=1}^{k-1} y_j + y_k \right] \\ &= \frac{1}{k} [(k-1) \bar{y}_{k-1} + y_k] \end{aligned}$$

10.1.3 Curve Fitting

In the recursive curve fitting problem, we measure data one sample at a time $(y_1, y_2 \ldots,)$ and want to find the best fit of a curve to the data. The curve that we want to fit to the data could be constrained to be linear or quadratic and so on.

Example: Suppose that we want to fit a straight line to a set of data points. The linear data fitting problem can be written as

$$\begin{aligned} y_k &= \theta_1 + \theta_2 t_k + \eta_k \\ \mathbb{E}[\eta_k] &= R_k \end{aligned}$$

t_k is the independent variable, y_k is the noisy data, and we want to find the linear relationship between y_k and t_k. In sum, we want to estimate the constants θ_1 and θ_2. The measurement matrix can be written as

$$\mathbf{X}_k = \begin{bmatrix} 1 & t_k \end{bmatrix}.$$

Then,

$$\mathbf{y}_k = \mathbf{X}_k \boldsymbol{\theta} + \boldsymbol{\eta}_k.$$

10.1.4 Python Implementation

```
class RecursiveLeastSquares(object):

    # theta0 - initial estimate used to initialize the estimator
    # P0 - initial estimation error covariance matrix
    # R  - covariance matrix of the measurement noise
    def __init__(self,theta0,P0,R)

        # initialize the values
        self.theta0=theta0
        self.P0=P0
        self.R=R

        # this variable is used to track the current time step k of the
    estimator
        # after every time step arrives, this variables increases for one
        # in this way, we can track the number of variblaes
        self.curr_step=0

        # this list is used to store the estimates xk starting from the initial
     estimate
        self.estimates=[]
        self.estimates.append(theta0)

        # this list is used to store the estimation error covariance matrices
    Pk
        self.est_error_cov=[]
        self.est_error_cov.append(P0)

        # this list is used to store the gain matrices Kk
        self.gainMatrices=[]

        # this list is used to store estimation error vectors
        self.errors=[]

```

```
32
33      # this function takes the current measurement and the current measurement
        matrix X
34      # and computes the estimation error covariance matrix, updates the estimate
        ,
35      # computes the gain matrix, and the estimation error
36      # it fills the lists self.estimates, self.est_error_cov, self.gainMatrices,
         and self.errors
37      # it also increments the variable curr_step for 1
38
39      # measurementValue (theta) - measurement obtained at the time instant k
40      # X - measurement matrix at the time instant k
41
42      def predict(self,measurementValue,X):
43          import numpy as np
44
45          # Compute the L matrix and its inverse
46          # K_k = P_{k-1}X_k^T(R_k+X_kP_{k-1}X_k^T)^{-1}
47          Lmatrix=self.R+np.matmul(X,np.matmul(self.est_error_cov[self.curr_step
        ],X.T))
48          LmatrixInv=np.linalg.inv(Lmatrix)
49          # Compute the gain matrix
50          gainMatrix=np.matmul(self.est_error_cov[self.curr_step],np.matmul(X.T,
        LmatrixInv))
51
52          # Compute the estimation error
53          # \theta_k = \theta_{k-1}+K_k (y_k-X_k\theta_{k-1})
54          error=measurementValue-np.matmul(X,self.estimates[self.curr_step])
55          # Compute the estimate
56          estimate=self.estimates[self.curr_step]+np.matmul(gainMatrix,error)
57
58          # Propagate the estimation error covariance matrix
59          # P_k = (I-K_k X_k)P_{k-1}(I-K_k X_k)^T+K_kR_kK_k^T
60          ImKc=np.eye(np.size(self.theta0),np.size(self.theta0))-np.matmul(
        gainMatrix,X)
61          error_cov=np.matmul(ImKc,self.est_error_cov[self.curr_step])
62
63          # add computed elements to the list
64          self.estimates.append(estimate)
65          self.est_error_cov.append(error_cov)
66          self.gainMatrices.append(gainMatrix)
67          self.errors.append(error)
68
69          # increment the current time step
70          self.curr_step=self.curr_step+1
```

10.2 Alternate Derivation of RLS

Suppose the training samples arrive one by one in the following sequence $\mathbf{x}_1, \ldots, \mathbf{x}_m, \mathbf{x}_{m+1}$, where $\mathbf{x}_{m+1}$ denotes the newly arrived sample vector. These samples can be projected onto the feature space by linear projection and expressed into a matrix $\mathbf{P}^T \in \mathbb{R}^{(d+1)\times(m+1)}$ as follows:

$$\mathbf{P}^T = [\mathbf{p}(\mathbf{x}_1), \ldots, \mathbf{p}(\mathbf{x}_{m+1})],$$

where $\mathbf{p}(\cdot) \in \mathbb{R}^{d+1}$. Subsequently, let

$$\mathbf{R}_{m+1} = \mathbf{P}^T\mathbf{P} + b\mathbf{I}$$
$$\mathbf{Q}_{m+1} = \mathbf{P}^T\mathbf{y}.$$

By separating the covariance of the newly arrived sample $p(\mathbf{x}_{m+1})$ from the remaining stack, we can write:

$$\begin{aligned}\mathbf{P}^T\mathbf{P} &= \sum_{i=1}^{m+1}\mathbf{p}(\mathbf{x}_i)\mathbf{p}(\mathbf{x}_i)^T \\ &= \sum_{i=1}^{m}\mathbf{p}(\mathbf{x}_i)\mathbf{p}(\mathbf{x}_i)^T + \mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T \\ &= \mathbf{P}_m^T\mathbf{P}_m + \mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T.\end{aligned}$$

Hence,

$$\begin{aligned}\mathbf{R}_{m+1} &= \mathbf{P}^T\mathbf{P} + b\mathbf{I} \\ &= \left(\mathbf{P}_m^T\mathbf{P}_m + \mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T\right) + b\mathbf{I} \\ &= \underbrace{\mathbf{P}_m^T\mathbf{P}_m + b\mathbf{I}}_{=\mathbf{R}_m} + \mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T \\ &= \mathbf{R}_m + \mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T\end{aligned}$$

Similarly,

$$\mathbf{Q}_{m+1} = \mathbf{Q}_m + \mathbf{p}(\mathbf{x}_{m+1})y_{m+1}$$

If the system is designed to forget the old training samples (*i.e.,* weighted averaging),

$$\begin{aligned}\mathbf{R}_{m+1} &= (1-\lambda)\mathbf{R}_m + \lambda\mathbf{p}(\mathbf{x}_{m+1})\mathbf{p}(\mathbf{x}_{m+1})^T, \\ \mathbf{Q}_{m+1} &= (1-\lambda)\mathbf{Q}_m + \lambda\mathbf{p}(\mathbf{x}_{m+1})y_{m+1},\end{aligned}$$

where $\lambda \in (0,1)$ is often called a *forgetting factor.*

Let $\mathbf{A} = \mathbf{R}_m, \mathbf{B} = p(\mathbf{x}_{m+1}), \mathbf{C} = 1$ (scalar), $\mathbf{D} = p(\mathbf{x}_{m+1})^T = \mathbf{p}^T$, then based on the matrix inversion lemma (Woodbury, 1950; Sherman and Morrison, 1950),

$$(\mathbf{A}+\mathbf{BCD})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}(\mathbf{C}^{-1} + \mathbf{D}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{D}\mathbf{A}^{-1},$$

we have

$$\begin{aligned}\mathbf{R}_{m+1}^{-1} &= \left[(1-\lambda)\mathbf{R}_m + \lambda\mathbf{p}\mathbf{p}^T\right]^{-1} \\ &= \frac{1}{1-\lambda}\mathbf{R}_m^{-1} - \frac{1}{1-\lambda}\mathbf{R}_m^{-1}\lambda\mathbf{p}\left(\mathbf{I} + \mathbf{p}^T\frac{\lambda}{1-\lambda}\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1}\mathbf{p}^T\frac{1}{1-\lambda}\mathbf{R}_m^{-1} \\ &= \frac{1}{1-\lambda}\mathbf{R}_m^{-1} - \frac{1}{(1-\lambda)^2}\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\left(\frac{1}{\lambda} + \frac{1}{1-\lambda}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1}.\end{aligned}$$

We can obtain

$$\mathbf{w}_{m+1} = \left(\mathbf{P}^T\mathbf{P} + b\mathbf{I}\right)^{-1}\mathbf{P}^T\mathbf{y} = \mathbf{R}_{m+1}^{-1}\mathbf{Q}_{m+1},$$

Substitute $\mathbf{R}_{m+1}^{-1}$ and $\mathbf{Q}_{m+1} = (1-\lambda)\mathbf{Q}_m + \lambda\mathbf{p}(\mathbf{x}_{m+1})y_{m+1}$:

$$\begin{aligned}\mathbf{w}_{m+1} &= \left[\frac{1}{1-\lambda}\mathbf{R}_m^{-1} - \frac{1}{(1-\lambda)^2}\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\left(\frac{1}{\lambda} + \frac{1}{1-\lambda}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1}\right]\left[(1-\lambda)\mathbf{Q}_m + \lambda y_{m+1}\mathbf{p}\right] \\ &= \underbrace{\mathbf{R}_m^{-1}\mathbf{Q}_m}_{=w_m} + \frac{1}{1-\lambda}\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\left(\frac{1}{\lambda} + \frac{1}{1-\lambda}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1}\mathbf{Q}_m + \frac{\lambda}{1-\lambda}\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} \\ &\quad - \frac{\lambda}{(1-\lambda)^2}\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\left(\frac{1}{\lambda} + \frac{1}{1-\lambda}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1}\mathbf{p}y_{m+1}\end{aligned}$$

Let

$$\begin{aligned} A &= \left(\frac{1}{\lambda} + \frac{1}{1-\lambda}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}\right)^{-1} \\ &= \frac{\lambda(1-\lambda)}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}, \end{aligned}$$

which is a constant. Then

$$\begin{aligned} w_{m+1} &= w_m - \frac{\mathbf{R}_m^{-1}\mathbf{p}}{(1-\lambda)^2} \cdot A \cdot \big((1-\lambda)\mathbf{p}^T w_m + \lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}y_{m+1}\big) + \frac{\lambda}{1-\lambda}\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} \\ &= w_m - \frac{\lambda\mathbf{R}_m^{-1}\mathbf{p}}{(1-\lambda)} \cdot \frac{1}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}\big((1-\lambda)\mathbf{p}^T w_m + \lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}y_{m+1}\big) + \frac{\lambda}{1-\lambda}\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} \\ &= w_m - \frac{\lambda\mathbf{R}_m^{-1}\mathbf{p}}{(1-\lambda)} \cdot \frac{1}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}\big((1-\lambda)\mathbf{p}^T w_m + \lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}y_{m+1}\big) \\ &\quad + \frac{\lambda}{(1-\lambda)} \cdot \frac{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} \text{ , since } \mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} \text{ is a scalar, we can put } \mathbf{R}_m^{-1}\mathbf{p} \text{ to the right} \\ &= w_m + \frac{\lambda}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)} \cdot \frac{1}{(1-\lambda)}\big(-(1-\lambda)\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T w_m - \lambda\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} \\ &\quad + \lambda\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p}y_{m+1} + (1-\lambda)\mathbf{R}_m^{-1}\mathbf{p}y_{m+1}\big) \\ &= w_m + \frac{\lambda}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)} \cdot \frac{1}{(1-\lambda)}\big(-(1-\lambda)\mathbf{R}_m^{-1}\mathbf{p}\mathbf{p}^T w_m + (1-\lambda)\mathbf{R}_m^{-1}\mathbf{p}y_{m+1}\big) \end{aligned}$$

Thus, the final recursive solution for the weight vector $\mathbf{w}_{m+1}$ is given by

$$\mathbf{w}_{m+1} = \mathbf{w}_m + \frac{\lambda\mathbf{R}_m^{-1}\mathbf{p}(y_{m+1} - \mathbf{p}^T\mathbf{w}_m)}{\lambda\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + (1-\lambda)}$$

Here, we note that λ controls the strength of update with respect to the accumulated solution with $\lambda \to 1$ having the strongest weight for newly arrived sample. When $\lambda = 0.5$ in , we have the following regularized recursive least squares solution:

$$w_{m+1} = w_m + \frac{\mathbf{R}_m^{-1}\mathbf{p}(y_{m+1} - \mathbf{p}^T w_m)}{\mathbf{p}^T\mathbf{R}_m^{-1}\mathbf{p} + 1}.$$

Chapter 11

Logistic Regression

11.1 Logistic Regression

Whereas linear regression maps inputs to $\mathbb{R}$, logistic regression predicts values in the bounded interval $[0, 1]$, letting us interpret the outputs as probabilities. We therefore pass the linear score through the *sigmoid* (logistic) function

$$\sigma(z) \;=\; \frac{1}{1+\exp(-z)}, \qquad z = \beta^{\top}\mathbf{x}.$$

The class probabilities are

$$P\{Y=1\,|\,X\} = \sigma(z), \qquad P\{Y=0\,|\,X\} = 1-\sigma(z).$$

We are going to use the Maximum Likelihood Estimation (MLE) to find the best parameter. The MLE is a method used in statistics to estimate the parameters of a probability distribution by maximizing a likelihood function. Essentially, MLE finds the parameter values that make the observed data most probable.

Let's first define the Likelihood Function: Based on the probability distribution of the data, write down the likelihood function. For a set of observations $X = \{x_1, x_2, \ldots, x_n\}$, and a parameter β, the likelihood function $L(\beta; X)$ represents the probability of observing the given data under the parameter β.

Since the likelihood can be a product of probabilities, it might be easier to work with the natural logarithm of the likelihood function, called the log-likelihood. This transforms the product into a sum, simplifying the computation:

$$\ell(\beta; X) = \log L(\beta; X)$$

Finally, to find the optimal parameter, find the parameter value $\hat{\beta}$ that maximizes the log-likelihood function.

For a dataset with n observations, the likelihood function is the product of the probabilities of observing the given outcomes. For logistic regression, the likelihood function $L(\beta; X, Y)$ is given by:

$$L(\beta; X, Y) = \prod_{i=1}^{n} P(Y_i|X_i, \beta)$$

Given the binary nature of Y, this can be written as:

$$L(\beta; X, Y) = \prod_{i=1}^{n} [P(Y_i = 1|X_i, \beta)]^{Y_i} [P(Y_i = 0|X_i, \beta)]^{1-Y_i}$$

Substituting the logistic function, we get:

$$L(\beta; X, Y) = \prod_{i=1}^{n} \left[\frac{1}{1 + \exp(-X_i\beta)}\right]^{Y_i} \left[1 - \frac{1}{1 + \exp(-X_i\beta)}\right]^{1-Y_i}$$

The negative log-likelihood for logistic regression is then given by

$$\text{NLL}(\beta) = -\sum_{i=1}^{N} y_i \ln \sigma(\beta^T \mathbf{x}) + (1 - y_i) \ln(1 - \sigma(\beta^T \mathbf{x})).$$

This is also called **cross-entropy** error function.

To compute the derivative of NLL, we first need to know the following tricks:

- The derivative of $\ln(x)$:
$$\frac{\partial}{\partial x} \ln(x) = \frac{1}{x}.$$
- The derivative of the sigmoid is given by:
$$\frac{\partial \sigma(z)}{\partial x} = \sigma(x)(1 - \sigma(x)).$$
- Finally, the chain rule of derivative. Suppose we are computing the derivative of a composite function $f(x) = u(v(x))$. The derivative of $f(x)$ is the derivative of $u(x)$ with respect to $v(x)$ times the derivative of $v(x)$ with respect to x.
$$\frac{\partial f}{\partial x} = \frac{\partial u}{\partial v} \frac{\partial v}{\partial x}$$

The derivative of the loss function w.r.t., a single weight w_j is given by

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\partial}{\partial w_j} - [\mathbf{y} \ln \sigma(\mathbf{wx} + \mathbf{b}) + (1 - \mathbf{y}) \ln(1 - \sigma(\mathbf{wx} + \mathbf{b}))] \\
&= -[\frac{\partial}{\partial w_j} y \ln \sigma(wx + b) + \frac{\partial}{\partial w_j}(1 - y) \ln(1 - \sigma(wx + b))] \\
&= -\frac{y}{\sigma(wx + b)} \frac{\partial}{\partial w_j} \sigma(wx + b) - \frac{1 - y}{1 - \sigma(wx + b)} \frac{\partial}{\partial w_j} [1 - \sigma(wx + b)] \\
&= -\left[\frac{y}{\sigma(wx + b)} - \frac{1 - y}{1 - \sigma(wx + b)}\right] \frac{\partial}{\partial w_j} \sigma(wx + b) \\
&= -\left[\frac{y - \sigma(wx + b)}{\sigma(wx + b)[1 - \sigma(wx + b)]}\right] \sigma(wx + b)[1 - \sigma(wx + b)] \frac{\partial \sigma(wx + b)}{\partial w_j} \\
&= -\left[\frac{y - \sigma(wx + b)}{\sigma(wx + b)[1 - \sigma(wx + b)]}\right] \sigma(wx + b)[1 - \sigma(wx + b)] x_j \\
&= -(y - \sigma(wx + b)) x_j \\
&= (\sigma(wx + b) - y) x_j.
\end{aligned}$$

[0] $\mathbb{I}(y_i = 1) = y_i$, because $y_i \in \{0, 1\}$ is a binary variable

Thus, the gradient of the cost function $J(\boldsymbol{\theta})$ with respect to the weights $\boldsymbol{\theta}$ is:

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{m}\mathbf{X}^T(\sigma(\mathbf{X}\boldsymbol{\theta}) - \mathbf{y})$$

This gradient is used in gradient descent to update the weights $\boldsymbol{\theta}$:

$$\boldsymbol{\theta} := \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}),$$

where α is the learning rate.

11.1.1 Another Interpretation

Logistic regression models *logit*s (log odds) through a linear model. For binary data, the goal is to model the probability p that one of two outcomes occurs. Recall that an ordinary linear regression model is not bounded. Thus, we will pass a linear model through a sigmoid function, which is also known as logistic function.

$$\sigma(z) = \frac{1}{1 + \exp^z},$$

where $z = wx + b$. The sigmoid function has the property

$$\sigma(-x) = 1 - \sigma(x).$$

The z is often called the logit. Note that the inverse of the sigmoid is the log of the odds ratio $\frac{p}{1-p}$.

The logit function is $\log\frac{p}{1-p}$, which varies between $-\infty$ and $+\infty$ as p varies between 0 and 1.

$$\log\frac{p}{1-p} = w_0x_0 + w_1x_1 + \cdots + w_nx_n.$$

Note that the logistic regression model assumes that the log-odds (also called the *logit*) of an observation y can be expressed as a linear function of the predictor variables. In this context, the logit function is referred to as the *link* function because it "links" the probability of an event to a linear combination of the predictors. The logit provides information about the ratio of two outcomes. For example, suppose an event has a probability of occurring of 60%. If a certain factor makes the event twice as likely to occur, the logit can be used to quantify this by comparing the probability of the event occurring to the probability of it not occurring.

Chapter 12

Bayesian Regression

12.1 Bayesian Regression

Chain rule: $P(A, B|C) = P(A|B, C)P(B|C)$

$$\begin{aligned} P(heads \mid D) &= \int_\theta P(heads, \theta \mid D) d\theta \\ &= \int_\theta P(heads \mid \theta, D) P(\theta \mid D) d\theta \\ &= \int_\theta \theta P(\theta \mid D) d\theta \\ &= E\left[\theta|D\right] \\ &= \frac{n_H + \alpha}{n_H + \alpha + n_T + \beta} \end{aligned}$$

12.2 Bayesian Regression

Bayesian regression is derived by combining the concepts of linear regression with Bayesian probability. In this note, we will derive Bayesian linear regression step-by-step, starting from a basic linear model and incorporating Bayesian inference.

12.3 Linear Regression Model

We assume a simple linear model:

$$y = X\beta + \epsilon,$$

where:

- y is the vector of observed responses (dependent variable),
- X is the matrix of observed features (independent variables),

- β is the vector of regression coefficients,
- $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$ is the noise term (normally distributed with mean 0 and variance σ^2).

This gives the likelihood function:

$$p(y|X, \beta, \sigma^2) = \mathcal{N}(y|X\beta, \sigma^2 I)$$

In the Bayesian framework, we treat the regression coefficients β as random variables with a prior distribution. Bayesian regression involves the following key elements:

- **Prior:** $p(\beta)$, which represents our belief about β before observing the data.
- **Likelihood:** $p(y|X, \beta)$, the likelihood of observing the data given the regression coefficients.
- **Posterior:** $p(\beta|y, X)$, which updates the prior belief based on the observed data.

According to Bayes' theorem, the posterior is:

$$p(\beta|y, X) = \frac{p(y|X, \beta)p(\beta)}{p(y|X)}$$

The term $p(y|X)$ is the marginal likelihood (evidence), which acts as a normalizing constant to ensure that the posterior is a valid probability distribution.

12.3.1 Prior on β

A common choice for the prior distribution on β is a Gaussian distribution:

$$p(\beta) = \mathcal{N}(\beta|\mu_0, \Sigma_0),$$

where μ_0 is the prior mean (our prior belief about β), and Σ_0 is the prior covariance matrix (representing the uncertainty in our prior belief).

12.3.2 Posterior Distribution

The posterior distribution of β is obtained by combining the likelihood with the prior using Bayes' theorem. The likelihood and prior are given by

$$\begin{aligned} p(y|X, \beta) &= \mathcal{N}(y|X\beta, \sigma^2 I) \\ p(\beta) &= \mathcal{N}(\beta|\mu_0, \Sigma_0). \end{aligned}$$

Since the posterior is proportional to the product of the prior and the likelihood (and applying properties of Gaussian distributions), we obtain the posterior distribution and it is also Gaussian:

$$p(\beta|y, X) = \mathcal{N}(\beta|\mu_n, \Sigma_n),$$

where:

- The **posterior mean** μ_n is given by:

$$\mu_n = \Sigma_n \left(\Sigma_0^{-1} \mu_0 + \frac{1}{\sigma^2} X^T y \right)$$

- The **posterior covariance** Σ_n is given by:

$$\Sigma_n = \left(\Sigma_0^{-1} + \frac{1}{\sigma^2} X^T X \right)^{-1}$$

We can find the best β by computing the highest posterior probability and it is called *maximum a posterior* (MAP) approach.

12.3.3 Prediction

Once we have the posterior distribution $p(\beta|y, X)$, we can make predictions on new data X_*.

The predictive distribution for the new output y_* given new input X_* is obtained by integrating over the posterior distribution of β:

$$p(y_*|X_*, y, X) = \int p(y_*|X_*, \beta) p(\beta|y, X) d\beta$$

Since both the likelihood and posterior are Gaussian, the predictive distribution is also Gaussian:

$$p(y_*|X_*, y, X) = \mathcal{N}(y_*|X_* \mu_n, X_* \Sigma_n X_*^T + \sigma^2 I)$$

In Bayesian regression, we incorporate prior beliefs about the regression coefficients through the prior distribution $p(\beta)$, and update this belief after observing data to obtain the posterior distribution $p(\beta|y, X)$. This method provides not only point estimates of the regression coefficients but also quantifies the uncertainty in these estimates through the posterior distribution.

Part III

Kernel Methods

Chapter 13

Introduction to Kernel Methods

13.1 Introduction

In machine learning a *kernel* is a function that measures similarity between two objects and, at the same time, implicitly maps those objects into (possibly very-high-dimensional) feature space without ever computing the coordinates of that space directly.

A basic idea of kernel machine learning algorithms is that we can make ML models non-linear by applying basis function (feature) transformations on the input space. For an input vector $\mathbf{x} \in \mathbb{R}^d$, do transformation $\mathbf{x} \rightarrow \phi(\mathbf{x}) \in \mathbb{R}^D$, where $D >> d$.

13.2 Kernel Trick

Kernel trick aims to avoid computing explicit feature transformations $\phi(\mathbf{x})$ by changing the entire ML algorithm to use only *inner products* of feature transformations $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$ which are computed directly using a *kernel* (rather than the feature transformations themselves.). Note that even the RBF kernel also can be expressed as an inner product.

This is contrast to many other ML algorithms that require explicit transformation of input data into feature vectors using a feature map, kernel methods directly compute similarity using a user-specified kernel function.

In other words, the terminology *kernel trick* simply refers to taking any algorithm the depends on the data only through inner products and replacing each inner product $\langle \mathbf{x}, \mathbf{x}' \rangle$ by a kernel value $k(\mathbf{x}, \mathbf{x}')$.

13.2.1 From Feature Transformations to Kernels

Instead of computing $\phi(\mathbf{x}_i), \forall i$, we pre-compute $\langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$ for all $\mathbf{x}_i$ and $\mathbf{x}_j$. Then we store the values in an $n \times n$ matrix K where $K_{ij} = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$. K is called the *kernel matrix* or *Gram matrix*.

Pre-computing the inner produce can be more efficient:

Approach	What we actually compute	Cost per evaluation
Explicit map	build $\varphi(x) \in \mathbb{R}^D$ then take $\langle \varphi(x), \varphi(z) \rangle$	$\mathcal{O}(D)$ (often gigantic)
Kernel trick	evaluate $K(x, z) = \langle \varphi(x), \varphi(z) \rangle$ directly	$\mathcal{O}(d)$, usually $d \ll D$

For instance, one might map $x \to (1, x, x^2)$ for quadratic features, $x \to (1, x, x^2, x^3)$ for cubic features, and so on.

$$y_t = \begin{cases} +1 & x_1^2 + x_1^2 \leq 1 \\ -1 & \text{otherwise} \end{cases}$$

For $\mathbf{x}[x_1, x_2]^T$, let $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

$$\begin{aligned} K(\mathbf{x}, \mathbf{x}') &= x_1^2 {x_1'}^2 + \sqrt{2}x_1x_2\sqrt{2}x_1'x_2' + x_2^2 {x_2'}^2 \\ &= (x_1x_1' + x_2x_2')^2 \\ &= \left\langle \mathbf{x}, \mathbf{x}' \right\rangle^2 \end{aligned}$$

13.3 Kernels

Formally, we can define that the kernel is the inner product of a fixed feature space mapping $\phi(\mathbf{x})$

$$k(\mathbf{x}, \mathbf{x}') = \left\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \right\rangle.$$

Hence, a kernel is a function $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. By the definition, a kernel function measures the similarity between data points. The kernel matrix is always an $n \times n$ matrix, whatever the nature of data. Also, it has a *modularity* between the choice of kernel function and the choice of learning algorithm. However, it tends to suffer from a poor scalability with respect to the dataset size.

Then, we can ask can any function be a kernel? The answer is no. To be a valid or well-defined kernel, it has to be *symmetric* (*i.e.,* $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}', \mathbf{x})$ for all $\mathbf{x}$ and $\mathbf{x}'$) and *positive semi-definite*. Also the feature map ϕ is a mapping from the input space to a feature space (*i.e.,* Hilbert space).

13.4 Hilbert Spaces

In functional analysis, $f(\cdot)$ denotes a function itself, while $f(x)$ represents the specific value that function takes at the input x.

Consider a function f that takes an input $\mathbf{x} = (x_1, x_2)$:

$$f(x) = f_1x_1 + f_2x_2 + f_3x_1x_2.$$

First we recall what is meant by a linear function. Given a vector space X over the reals, a function

$$f : X \longrightarrow \mathbb{R}$$

is linear if $f(\alpha\mathbf{x}) = \alpha f(\mathbf{x})$ and $f(\mathbf{x} + \mathbf{z}) = f(\mathbf{x}) + f(\mathbf{z}), \forall \mathbf{x}, \mathbf{z} \in X, \alpha \in \mathbb{R}$.

Inner product space A vector space X over the reals R is an *inner product space* if there exists a real-valued symmetric bilinear map $\langle \cdot, \cdot \rangle$, that satisfies

$$\langle \mathbf{x}, \mathbf{x} \rangle \geq 0.$$

The bilinear map is known as the inner, dot or scalar product. Furthermore we will say the inner product is strict if

$$\langle \mathbf{x}, \mathbf{x} \rangle = 0 \iff \mathbf{x} = \mathbf{0}.$$

Given a strict inner product space, we can define a norm on the space X by

$$|\mathbf{x}|_2 = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}.$$

The associated metric or distance between two vectors is defined as $d(\mathbf{x}, \mathbf{z}) = |\mathbf{x} - \mathbf{z}|_2$. For the vector space $\mathbb{R}^n$ the standard inner product is given by

$$\langle \mathbf{x}, \mathbf{z} \rangle = \sum_{i=1}^{n} x_i, z_i.$$

An inner product space is sometimes referred to as a *Hilbert space*, though most researchers require the additional properties of completeness and separability, as well as sometimes requiring that the dimension be infinite. We give a formal definition.

Hilbert Space A Hilbert Space $\mathcal{F}$ is an inner product space with the additional properties that it is *separable* and *complete*. Completeness refers to the property that every Cauchy sequence $\{h_n\}_{n \geq 1}$ of elements of $\mathcal{F}$ converges to an element $h \in \mathcal{F}$, where a Cauchy sequence is one satisfying the property that

$$\sup_{m > n} |h_n - h_m| \to 0, \text{ as } n \to \infty.$$

A space$\mathcal{F}$ is separable if for any $\epsilon > 0$ there is a finite set of elements $h_1, \ldots, h_N$ of $\mathcal{F}$ such taht for all $h \in \mathcal{F}$

$$\min_i |h_i - h| < \epsilon.$$

For instance, Let X be the set of all countable sequences of real numbers $\mathbf{x} = (x_1, \ldots, x_n, \ldots)$, such that the sum

$$\sum_{i=1}^{\infty} x_i^2 < \infty,$$

with the inner product between two sequences $\mathbf{x}$ and $\mathbf{y}$ defined by

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^{\infty} x_i y_i.$$

This is the space known as L_2.

- A vector space is just a collection of objects you can add and scale (*e.g.,* $\mathbf{v} + \mathbf{w}$,$3\mathbf{v}$) and all the usual algebra rules hold.

- An inner product $\langle , \cdot, \cdot \rangle$ on a vector space is a generalisation of the dot product. It must satisfy
  - Bilinearity$\langle a\mathbf{v} + b\mathbf{w}, \mathbf{z}\rangle = a\langle \mathbf{v}, \mathbf{z}\rangle + b\langle \mathbf{w}, \mathbf{z}\rangle$ (and similarly in the second slot).
  - Symmetry$\langle \mathbf{v}, \mathbf{w}\rangle = \langle \mathbf{w}, \mathbf{v}\rangle$.
  - Positive-definiteness$\langle \mathbf{v}, \mathbf{v}\rangle \geq 0$ with equality only when $\mathbf{v} = 0$.
- A metric space is *complete* when every Cauchy sequence actually converges to a limit inside the space.
  - Analogy: rational numbers $\mathbb{Q}$ are not complete as Cauchy sequences like $3, 3.1, 3.14, 3.141, \ldots$ hover toward π, which is missing from $\mathbb{Q}$. The reals $\mathbb{R}$ are complete.
  - Completeness is crucial for analysis: it guarantees limits, projections, series expansions (*e.g.,* Fourier), and many theorems work internally without you stepping outside the space.

13.5 Properties

Given a finite subset $\mathcal{S} = \{\mathbf{x}_1, \ldots, \mathbf{x}_l\}$ of an input space $\mathbf{X}$, a kernel $\kappa(\mathbf{x}, \mathbf{z})$ and a feature map ϕ into a feature space F satisfying

$$\kappa \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle ,$$

let $\phi(S) = \{\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_l)\}$ be the image of S under the map ϕ. Hence $\phi(S)$ is a subset of the inner product of space F. Then the kernel matrix $\mathbf{K}$ of kernel evaluations between all pairs of elements of S is given by

$$\mathbf{K}_{ij} = \kappa \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle , \quad i, j = 1, \ldots, l$$

Working in a kernel-defined feature space means that we are not able to explicitly represent points. For example the image of an input point $\mathbf{x}$ is $\phi(\mathbf{x})$, but we do not have access to the components of this vector, only to the evaluation of inner products between this point and the images of other points. Despite this handicap there is a surprising amount of useful information that can be gleaned about $\phi(\mathbf{S})$.

For two data points the transformed kernel $\hat{\kappa}$ is given by

$$\begin{aligned}\kappa(\mathbf{x}, \mathbf{z}) &= \left\langle \hat{\phi}(\mathbf{x}), \hat{\phi}(\mathbf{z}) \right\rangle = \left\langle \frac{\phi(\mathbf{x})}{\|\phi(\mathbf{x})\|}, \frac{\phi(\mathbf{z})}{\|\phi(\mathbf{z})\|} \right\rangle = \frac{\phi(\mathbf{x})\phi(\mathbf{z})}{\|\phi(\mathbf{x})\|\|\phi(\mathbf{z})\|} \\ &= \frac{\kappa(\mathbf{x}, \mathbf{z})}{\sqrt{\kappa(\mathbf{x}, \mathbf{x})\kappa(\mathbf{z}, \mathbf{z})}}\end{aligned}$$

```
% original kernel matrix stored in variable K
% output uses the same variable K
% D is a diagonal matrix storing the inverse of the norms
import numpy as np

# Example kernel matrix (must be symmetric with  n o n negative  diagonal entries
    )
K = np.array([[4.0, 2.0, 2.0],
```

```
                [2.0, 3.0, 0.5],
                [2.0, 0.5, 1.0]])

D = np.diag(1.0 / np.sqrt(np.diag(K)))

# Normalize the kernel
K = D @ K @ D            # same variable name as in MATLAB code
```

We can also evaluate the norms of linear combinations of images in the feature space. For example, we have

$$\begin{aligned}\left\|\sum_{i=1}^{l}\alpha_i\phi(\mathbf{x}_i)\right\|^2 &= \left\langle\sum_{i=1}^{l}\alpha_i\phi(\mathbf{x}_i),\sum_{i=j}^{l}\alpha_j\phi(\mathbf{x}_j)\right\rangle \\ &= \sum_{i=1}^{l}\alpha_i\sum_{i=j}^{l}\alpha_j\left\langle\phi(\mathbf{x}),\phi(\mathbf{z})\right\rangle \\ &= \sum_{i,j=1}^{l}\alpha_i\alpha_j\kappa(\mathbf{x},\mathbf{z}).\end{aligned}$$

A special case of the norm is the length of the line joining two images $\phi(\mathbf{x})$ and $\phi(\mathbf{z})$, $which can be computed as$

13.6 Kernel Regression

Recall that

$$\begin{aligned}(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})\boldsymbol{\theta} &= (\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} \\ (\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})\boldsymbol{\theta} &= \mathbf{X}^T\mathbf{y} \\ \boldsymbol{\theta} &= \lambda^{-1}\mathbf{I}(\mathbf{X}^T\mathbf{y}-\mathbf{X}^T\mathbf{X}\boldsymbol{\theta}) \\ &= \mathbf{X}^T\underbrace{\lambda^{-1}(\mathbf{y}-\mathbf{X}\boldsymbol{\theta})}_{=\alpha} \\ &= \mathbf{X}^T\alpha\end{aligned}$$

This tells us that $\boldsymbol{\theta}$ is a linear combination of $\boldsymbol{X}$ with α. Then,

$$\begin{aligned}\lambda\alpha &= (\mathbf{y}-\mathbf{X}\boldsymbol{\theta}) \\ &= (\mathbf{y}-\mathbf{X}\mathbf{X}^T\alpha) \\ \mathbf{y} &= (\mathbf{X}\mathbf{X}^T\alpha+\lambda\alpha) \\ \alpha &= (\mathbf{X}\mathbf{X}^T+\lambda)^{-1}\mathbf{y} \\ &= (\mathbf{G}+\lambda)^{-1}\mathbf{y}.\end{aligned}$$

$$\hat{\boldsymbol{\theta}} = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T+\lambda\mathbf{I})^{-1}\mathbf{y}.$$

By substituting into $\hat{y}(\mathbf{x}') = \hat{\boldsymbol{\theta}}^T\mathbf{x}' = (\mathbf{x}')^T\hat{\boldsymbol{\theta}}$ gives

$$\hat{y}(\mathbf{x}') = (\mathbf{x}')^T\hat{\boldsymbol{\theta}} = (\mathbf{x}')^T\mathbf{X}^T(\mathbf{X}\mathbf{X}^T+\lambda\mathbf{I})^{-1}\mathbf{y}.$$

The prediction depends on the data only though inner products, since

$$(\mathbf{x}')^T\mathbf{X}^T = \begin{bmatrix} \langle \mathbf{x}', \mathbf{x}_1 \rangle \\ \vdots \\ \langle \mathbf{x}', \mathbf{x}_n \rangle \end{bmatrix}, \quad \mathbf{X}\mathbf{X}^T = \begin{bmatrix} \langle \mathbf{x}_1, \mathbf{x}_1 \rangle & \cdots & \langle \mathbf{x}_1, \mathbf{x}_n \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{x}_n, \mathbf{x}_1 \rangle & \cdots & \langle \mathbf{x}_n, \mathbf{x}_n \rangle \end{bmatrix},$$

The kernel trick replaces the inner products by kernel evaluations, which can be represented as follows:

$$\hat{y}(\mathbf{x}') = k(\mathbf{x}')(K + \lambda \mathbf{I})^{-1}\mathbf{y},$$

where

$$k(\mathbf{x}') = \begin{bmatrix} k(\mathbf{x}', \mathbf{x}_1) \\ \vdots \\ k(\mathbf{x}', \mathbf{x}_n) \end{bmatrix} \quad K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix},$$

- The estimate $\hat{y}$ is a weighted sum of the previously observed outputs, $\mathbf{y}$. The more similar $\mathbf{x}'$ is to the corresponding $\mathbf{x}_t$ (*i.e.,* the higher value of $k(\mathbf{x}, \mathbf{x}')$), the more weight is given to that $\mathbf{y}$.
- Note that we have turned the original learning problem that had d parameters into one that has n parameters (*i.e.,* the number of data samples).

13.6.1 Non-Parametric Regression

Kernel methods corresponding to infinite-dimensional $\phi(\mathbf{x})$ can usually be considered as **non-parametric**. For instance, 1-D case can be considered as a joining the dots by interpolation.

13.7 From Feature Transformations to Kernels

Instead of computing $\phi(\mathbf{x}_i), \forall i$, we pre-compute $\langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$ for all $\mathbf{x}_i$ and $\mathbf{x}_j$. Then we store the values in an $n \times n$ matrix K where $K_{ij} = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$. K is called the kernel matrix or Gram matrix.

Computing $\phi(\mathbf{x}_i)$ is $\mathcal{O}(2^d) \times n = \mathcal{O}(2^d n)$. On the other hand, pre-computing the inner products can be more efficient as follows:

$$\begin{aligned} \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle &= \phi(\mathbf{x})^T \phi(\mathbf{x}') \\ &= \prod_{k=1}^{d} (1 + x_k x'_k). \end{aligned}$$

This takes $\mathcal{O}(d)$ and we can compute the entire kernel matrix K in $\mathcal{O}(dn^2)$.

Note that all kernel methods are non-parametric models as we need to keep training data to be able to compute the kernel values between new test inputs and the training inputs.

13.8 Kernels

$k(\cdot,\cdot)$ is a valid or well-defined kernel, if the function $k(\mathbf{x},\mathbf{x}')$ is both

- Symmetric: $k(\mathbf{x},\mathbf{x}') = k(\mathbf{x}',\mathbf{x})$ for all $\mathbf{x},\mathbf{x}'$.
- Positive semi-definite: $k(\cdot,\cdot)$ is PSD if for all finite subsets $\{\mathbf{x}_1,\ldots,\mathbf{x}_m\}$, $\mathbf{x}_i \in \mathcal{X}$, K is a PSD matrix.

Note that

- A matrix $A \in \mathbb{R}^{m\times m}$ is PSD iff $\forall \mathbf{q} \in \mathbb{R}^m$ the following holds: $\mathbf{q}^T A\mathbf{q} \geq 0$.
- A symmetric matrix $A \in \mathbb{R}^{m\times m}$ is PSD iff all eigenvalues λ of A are non-negative.
- A symmetric matrix A is PSD if all its upper left sub-matrices have non-negative determinants.

For symmetric matrices all of the above are equivalent.

Some of the most popular kernels are

- Linear kernel: $k(\mathbf{x},\mathbf{x}') = \mathbf{x}^T\mathbf{x}'$
- Polynomial kernel: $k(\mathbf{x},\mathbf{x}') = (1+\mathbf{x}^T\mathbf{x}')^{\tilde{d}}$, where $\tilde{d}$ is the degree of the polynomial

Note that some kernels such as the RBF kernel have an infinite-dimensional feature space transformation. Hence, it is impossible to compute the feature space transformation explicitly. The RBF kernel is given by

$$k(\mathbf{x},\mathbf{x}') = \exp(-\gamma\|\mathbf{x}-\mathbf{x}'\|^2)$$

Let, $\gamma = \frac{1}{2}$,

$$\begin{aligned}
k(\mathbf{x},\mathbf{x}') &= \exp(-\frac{1}{2}\|\mathbf{x}-\mathbf{x}'\|^2) \\
&= \exp\Big[-\frac{1}{2}\langle \mathbf{x}-\mathbf{x}', \mathbf{x}-\mathbf{x}'\rangle\Big] \\
&= \exp\Big[-\frac{1}{2}\langle \mathbf{x}, \mathbf{x}-\mathbf{x}'\rangle - \langle \mathbf{x}', \mathbf{x}-\mathbf{x}'\rangle\Big] \\
&= \exp\Big[-\frac{1}{2}\big(\|\mathbf{x}\|^2 + \|\mathbf{x}'\|^2 - 2\langle \mathbf{x}, \mathbf{x}'\rangle\big)\Big] \\
&= C\exp\langle \mathbf{x}, \mathbf{x}'\rangle \\
&= C\sum_{n=0}^{\infty}\frac{\langle \mathbf{x}, \mathbf{x}'\rangle}{n!} \\
&= C\sum_{n=0}^{\infty}\frac{k_{\text{poly}}(\mathbf{x},\mathbf{x}')}{n!}
\end{aligned}$$

The second to last step is by Taylor expansion of e^x.

13.8.1 Some Intuitions

Let $y = f(\mathbf{x}) + \epsilon$. Then f does not vary a lot if $\mathbf{x}$, $\mathbf{x}'$ are close enough. This can be modeled by the co-variance of the y's.

Let's represent the co-variance of the outputs in terms of the co-variance of the inputs.

$$cov(y, y') = k(\mathbf{x}, \mathbf{x}') + \underbrace{\sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'}}_{\text{noise term}} .$$

As y is a function values of $f(\mathbf{x})$, the kernel function can be viewed as an extension of the covariance matrix Σ of random vectors to the covariance of (random) functions.

Chapter 14

Gaussian Process

14.1 Introduction

A *Gaussian process* (GP) is a probability distribution over possible functions that fit a set of points fully specified by a mean and covariance function (posterior over f, function space view). It is a generalization of the Gaussian probability distribution. Whereas a probability distribution describes random variables which are scalars or vectors (for multivariate distributions), a stochastic process governs the properties of functions.

It means that GPs don't give you a single function to fit data. They will give you an entire distribution of possible functions. More formally, GPs define **distributions over functions** $f(x)$ of which the distribution is defined by a mean function $m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$ and positive definite covariance function $k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))]$, which tells us how points are related to each other (*i.e., kernel*). Thus, it is a distribution over functions whose shape is defined by the kernel:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')).$$

Let's say we have points then GPs assume that the function values of the points follow a multivariate Gaussian distribution. For example, we have observations $\boldsymbol{X} = \{x_1, \ldots, x_5\}$, then we have

$$\begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_5) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(x_1) \\ m(x_2) \\ \vdots \\ m(x_5) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_5) \\ \vdots & \ddots & \vdots \\ k(x_5, x_1) & \cdots & k(x_5, x_5) \end{bmatrix} \right),$$

More formally, let' say we have estimated functions $\mathbf{f} = [f(x_1), \ldots, f(x_n)]$ with these observations. Now say we have some new points $\mathbf{X}_*$ where we want to predict $f(\mathbf{X}_*)$.

The joint distribution of $\mathbf{f}$ and $\mathbf{f}_*$ can be modeled as:

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m(\mathbf{X}) \\ m(\mathbf{X}_*) \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right),$$

where $m(X) = [m(x_1), \ldots, m(x_n)]$ and

$$\begin{aligned}\mathbf{K} &= \kappa(\mathbf{X}, \mathbf{X}) \\ \mathbf{K}_* &= \kappa(\mathbf{X}, \mathbf{X}_*) \\ \mathbf{K}_{**} &= \kappa(\mathbf{X}_*, \mathbf{X}_*).\end{aligned}$$

The mean is assumed to be $(m(\mathbf{X}), m(\mathbf{X}_*)) = 0$.

While this equation describes the joint probability distribution $P(\mathbf{f}, \mathbf{f}_*|\mathbf{X}, \mathbf{X}_*)$ over $\mathbf{f}$ and $\mathbf{f}_*$ in regressions, we need the conditional distribution $P(\mathbf{f}_*|\mathbf{f}, \mathbf{X}, \mathbf{X}_*)$ for a prediction. The conditional distribution can be achieved by the Marginal and conditional distributions of MVN theorem:

Theorem 1 *Marginals and conditionals of an MVN: A random vector* $\mathbf{X}$ *follows a multivariate normal distribution:*

$$\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\mathbf{X}$ *can be partitioned as:*

$$\mathbf{X} = \begin{bmatrix}\mathbf{X}_1 \\ \mathbf{X}_2\end{bmatrix}$$

with corresponding partitions of the mean vector $\boldsymbol{\mu}$ *and the covariance matrix* $\boldsymbol{\Sigma}$*:*

$$\boldsymbol{\mu} = \begin{bmatrix}\boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2\end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix}\boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22}\end{bmatrix}, \quad \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1} = \begin{bmatrix}\boldsymbol{\Lambda}_{11} & \boldsymbol{\Lambda}_{12} \\ \boldsymbol{\Lambda}_{21} & \boldsymbol{\Lambda}_{22}\end{bmatrix},$$

Then, the marginal distribution of $\mathbf{X}_1$ *and* $\mathbf{X}_2$ *are given by*

$$\begin{aligned}\mathbf{X}_1 &\sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}) \\ \mathbf{X}_2 &\sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})\end{aligned}$$

Subsequently, the (posteriror) conditional distribution of $\mathbf{X}_1$ *given* $\mathbf{X}_2$ *is:*

$$\mathbf{X}_1|\mathbf{X}_2 = \mathbf{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}', \boldsymbol{\Sigma}'),$$

where the conditional mean $\boldsymbol{\mu}_{1|2}$ *and the conditional covariance* $\boldsymbol{\Sigma}_{1|2}$ *are given by:*

$$\begin{aligned}\boldsymbol{\mu}' &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ \boldsymbol{\Sigma}' &= \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}\end{aligned}$$

Note that $\boldsymbol{\Sigma}'$ does no depend on $\mathbf{x}_2$. It doesn't hold for general (non-Gaussian) random variables. By using the theorem, we get

$$\mathbf{f}_*|\mathbf{f}, \mathbf{X}, \mathbf{X}_* \sim \mathcal{N}(\mathbf{K}_*^T\mathbf{K}^{-1}\mathbf{f}, \mathbf{K}_{**} - \mathbf{K}_*^T\mathbf{K}^{-1}\mathbf{K}_*)$$

In practice, we typically have noisy estimations of target functions, $y = f(x) + \epsilon$. By assuming the i.i.d., Gaussian noise with variance σ_n^2, the prior on these noisy observations then becomes $cov(y) = \mathbf{K} + \sigma_n^2\mathbf{I}$. The joint distribution of the observed target values and the function values at the test locations under the prior as

$$\begin{bmatrix}\mathbf{y} \\ \mathbf{f}_*\end{bmatrix} \sim \mathcal{N}\left[\mathbf{0}, \begin{bmatrix}\mathbf{K} + \sigma_n^2\mathbf{I} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**}\end{bmatrix}\right]$$

14.2 Regression using Gaussian Process

- A set of input points $X = \{x_1, x_2, \ldots, x_n\}$ (*i.e.,* training data).
- A set of corresponding output values $y = \{y_1, y_2, \ldots, y_n\}$.

We assume that the output values are generated by some unknown function $f(x)$ with some Gaussian noise ϵ:

$$y = f(X) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

The goal is to predict the value of the function $f(x_*)$ at a new input point x_*.

We assume that the function $f(x)$ is drawn from a **Gaussian Process**:

$$f(x) \sim \mathcal{GP}(m(x), k(x, x')),$$

where:

- $m(x)$ is the mean function (usually assumed to be 0 for simplicity).
- $k(x, x')$ is the covariance function (or kernel), which encodes assumptions about the smoothness of the function.

The actual observations $y = f(x) + \epsilon$ include Gaussian noise ϵ, which is typically assumed to have zero mean and variance σ_n^2.

To predict the function value $f_* = f(x_*)$ at a new point x_*, we use the **posterior distribution** over the function, conditioned on the observed data X and y. This leads to two main equations:

- Posterior Mean (Prediction):

$$\mathbb{E}[f_*] = K(X, x_*)^\top [K(X, X) + \sigma_n^2 I]^{-1} y$$

- Posterior Variance (Uncertainty):

$$\text{Var}[f_*] = K(x_*, x_*) - K(X, x_*)^\top [K(X, X) + \sigma_n^2 I]^{-1} K(X, x_*)$$

These equations give us the mean and variance of the predictive distribution for the function value at the new point x_*.

Example: First, choose a covariance function (*i.e.,* Kernel). The kernel function $k(x, x')$ is crucial in defining the relationship between different input points. Some commonly used kernels are:

Squared Exponential (RBF) Kernel:

$$k(x, x') = \sigma_f^2 \exp\left(-\frac{(x - x')^2}{2l^2}\right),$$

where l is the length scale and σ_f^2 is the signal variance. The kernel function governs the smoothness and behavior of the GP, so selecting an appropriate kernel is important.

Subsequently, compute the covariance matrices:

- Covariance Matrix for Training Points: $K(X, X)$

$$K(X,X) = \begin{bmatrix} k(x_1,x_1) & k(x_1,x_2) & \dots & k(x_1,x_n) \\ k(x_2,x_1) & k(x_2,x_2) & \dots & k(x_2,x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n,x_1) & k(x_n,x_2) & \dots & k(x_n,x_n) \end{bmatrix}$$

- Covariance Between Training Points and Test Point: $K(X, x_*)$

$$K(X,x_*) = \begin{bmatrix} k(x_1,x_*) \\ k(x_2,x_*) \\ \vdots \\ k(x_n,x_*) \end{bmatrix}$$

- Covariance at the Test Point: $K(x_*, x_*) = k(x_*, x_*)$

Then, compute the posterior mean and variance by Using the posterior mean and posterior variance equations from earlier, compute:

- The mean prediction $\mathbb{E}[f_*]$ at the test point x_*.
- The uncertainty $\text{Var}[f_*]$ at x_*.

This gives the complete predictive distribution for the function value at x_*.

14.3 Time Complexity

One drawback of Gaussian processes is that it scales very badly with the number of observations N. It takes $O(N^3)$ time, since we need to compute the inverse of the kernel matrix.

14.4 Example

We observe two training points in $\mathbb{R}^2$:

$$X = \{(0,0),(1,1)\}, \quad y = \{1,2\}.$$

We want to predict the function value at a new test point:

$$x_* = (0,1).$$

We use the squared exponential (RBF) kernel for 2D inputs:

$$k(x,x') = \exp\left(-\frac{\|x-x'\|^2}{2\ell^2}\right), \quad \ell = 1.$$

Assume zero mean and no noise ($\sigma_n^2 = 0$).

Compute covariance matrices Training covariance:

$$K(X,X) = \begin{bmatrix} k((0,0),(0,0)) & k((0,0),(1,1)) \\ k((1,1),(0,0)) & k((1,1),(1,1)) \end{bmatrix}.$$

Compute distances:

- $\|(0,0)-(0,0)\|^2 = 0 \quad \Rightarrow k = 1.$
- $\|(0,0)-(1,1)\|^2 = 1^2+1^2 = 2 \quad \Rightarrow k = e^{-1} = 0.3679.$
- $\|(1,1)-(1,1)\|^2 = 0 \quad \Rightarrow k = 1.$

So:

$$K = \begin{bmatrix} 1 & 0.3679 \\ 0.3679 & 1 \end{bmatrix}.$$

Cross-covariance $K(X, x_*)$:

Distances:

- $\|(0,0)-(0,1)\|^2 = 1 \quad \Rightarrow k = e^{-0.5} = 0.6065.$
- $\|(1,1)-(0,1)\|^2 = 1 \quad \Rightarrow k = e^{-0.5} = 0.6065.$

So:

$$K(X, x_*) = \begin{bmatrix} 0.6065 \\ 0.6065 \end{bmatrix}.$$

Test covariance:

$$K(x_*, x_*) = 1.$$

Posterior mean

$$\mathbb{E}[f_*] = K(X, x_*)^\top K(X,X)^{-1} y.$$

Compute K^{-1}. For a 2×2 symmetric matrix:

$$K^{-1} = \frac{1}{1-(0.3679)^2} \begin{bmatrix} 1 & -0.3679 \\ -0.3679 & 1 \end{bmatrix}.$$

Denominator: $1 - 0.1353 = 0.8647$. So:

$$K^{-1} \approx \begin{bmatrix} 1.156 & -0.425 \\ -0.425 & 1.156 \end{bmatrix}.$$

Now multiply:

$$K^{-1} y = \begin{bmatrix} 1.156 & -0.425 \\ -0.425 & 1.156 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

$$= \begin{bmatrix} 1.156(1) - 0.425(2) \\ -0.425(1) + 1.156(2) \end{bmatrix} = \begin{bmatrix} 0.306 \\ 1.887 \end{bmatrix}.$$

Now compute mean:

$$\mathbb{E}[f_*] = [0.6065 \;\; 0.6065] \begin{bmatrix} 0.306 \\ 1.887 \end{bmatrix}.$$

$$= 0.6065(0.306 + 1.887) = 1.33.$$

Posterior mean:

$$\mathbb{E}[f(0,1)] \approx 1.33.$$

Posterior variance

$$\text{Var}[f_*] = K(x_*, x_*) - K(X, x_*)^\top K(X, X)^{-1} K(X, x_*).$$

First compute:

$$v = K^{-1} K(X, x_*) = \begin{bmatrix} 1.156 & -0.425 \\ -0.425 & 1.156 \end{bmatrix} \begin{bmatrix} 0.6065 \\ 0.6065 \end{bmatrix}.$$

$$= \begin{bmatrix} (1.156 - 0.425)(0.6065) \\ (-0.425 + 1.156)(0.6065) \end{bmatrix} = \begin{bmatrix} 0.443 \\ 0.443 \end{bmatrix}.$$

Now:

$$K(X, x_*)^\top v = [0.6065 \;\; 0.6065] \begin{bmatrix} 0.443 \\ 0.443 \end{bmatrix}.$$

$$= 0.6065(0.443 + 0.443) = 0.537.$$

So:

$$\text{Var}[f_*] = 1 - 0.537 = 0.463.$$

Posterior variance

$$\text{Std}[f(0,1)] \approx \sqrt{0.463} \approx 0.68.$$

For training data $((0,0),1),((1,1),2)$ and test point $(0,1)$:

$$f(0,1) \sim \mathcal{N}(1.33,\ 0.68^2).$$

Chapter 15

Support Vector Machine

Support Vector Machines (SVMs) are among the most effective and versatile tools in machine learning, widely used for various tasks. SVMs work by finding the optimal boundary, or hyperplane, that separates different classes of data with the maximum margin, making them highly reliable for classification, especially with complex datasets.

What truly sets SVMs apart is their ability to handle both linear and non-linear data through the *kernel trick*, allowing them to adapt to a wide range of problems with impressive accuracy. In this blog post, we'll delve into how SVMs work and gently explore the mathematical foundations behind their powerful performance.

15.1 Decision Boundary with Margin

A hyperplane(or decision surface) is used to separate data points belonging to different classes. The goal of SVM is to find the optimal separating hyperplane. However, what is the optimal separating hyperplanes? **The optimal hyperplane is the one which maximizes the distance from the hyperplane to the nearest data point of any class. Support vectors are the data points that lie closest to the hyperplane**. The distance is referred to as the *margin*. SVMs maximize the margin around the separating hyperplane.

The equation of a hyperplane in $\mathbb{R}^p$ can be expressed as:

$$\mathbf{w} \cdot \mathbf{x} + b = 0.$$

Here, $\mathbf{w}$ is the normal vector to the hyperplane. It is clear when we set $b = \mathbf{w} \cdot \mathbf{x}_0$

$$\mathbf{w}(\mathbf{x} - \mathbf{x}_0) = 0.$$

Let's consider a simple scenario, where training data is linearly separable:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in \mathbb{R}^p,\ y_i \in \{-1, 1\}\}_{i=1}^{N}.$$

Then, we can build two supporting hyperplanes, which separate the data with no points between them:

- $H_1 : \mathbf{w} \cdot \mathbf{x} + b = 1$

- $H_2 : \mathbf{w} \cdot \mathbf{x} + b = -1$

All samples have to satisfy one of two constraints:

1. $\mathbf{w} \cdot \mathbf{x} + b \geq 1$
2. $\mathbf{w} \cdot \mathbf{x} + b \leq -1$

For instance, if we set $\mathbf{w} = (0.5, 0.5)$, $b = -3$, then $\mathbf{x} = (4, 5)$ will be at H_1 and $\mathbf{x} = (2, 1)$ at H_2. Collectively, these constraints can be combined into a single expression:

$$y \cdot (\mathbf{w} \cdot \mathbf{x} + b) \geq 1.$$

To maximize the margin, we can consider a unit vector $\mathbf{u} = \frac{\mathbf{w}}{\|\mathbf{w}\|}$, which is perpendicular to the hyperplanes and a point $\mathbf{x}_0$ on H_2. If we scale $\mathbf{u}$ from $\mathbf{x}_0$, we get $\mathbf{z} = \mathbf{x}_0 + \gamma\mathbf{u}$ and we assume that $\mathbf{z}$ reaches at H_1. Then, $\mathbf{w} \cdot \mathbf{z} + b = 1$. This is equivalent to

$$\begin{aligned}
\mathbf{w} \cdot (\mathbf{x}_0 + \gamma\mathbf{u}) + b &= 1 \\
\mathbf{w}\mathbf{x}_0 + \mathbf{w}\gamma\frac{\mathbf{w}}{\|\mathbf{w}\|} + b &= 1 \\
\mathbf{w}\mathbf{x}_0 + \gamma\|\mathbf{w}\| + b &= 1 \\
\mathbf{w}\mathbf{x}_0 + b &= 1 - \gamma\|\mathbf{w}\|
\end{aligned}$$

As $\mathbf{x}_0$ is on H_2, we get $\mathbf{w}\mathbf{x}_0 + b = -1$. Finally, we obtain

$$\begin{aligned}
-1 &= 1 - \gamma\|\mathbf{w}\| \\
\gamma &= \frac{2}{\|\mathbf{w}\|}.
\end{aligned}$$

Note that the scaled unit vector $\gamma\mathbf{u}$'s magnitude is γ. Thus, the maximization of margin is equivalent to maximize γ. To maximize γ (*i.e.,* margin), we have to minimize $\|\mathbf{w}\|$. Thus, finding the optimal hyperplane reduces to solving the following optimization problem:

$$\begin{aligned}
&\min\|\mathbf{w}\|, \text{ subject to} \\
&y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \quad \forall i.
\end{aligned}$$

Equivalently,

$$\begin{aligned}
&\min \frac{1}{2}\|\mathbf{w}\|^2, \text{ subject to} \\
&y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \quad \forall i.
\end{aligned}$$

Now, we have *convex quadratic optimization problem*. The solution of this problem gives us the optimal hyperplane that maximizes the margin (*c.f.,* §15.3). However, in practice, the data may not be perfectly separable. To address this, we introduce a *soft margin* that allows for some misclassification. This is done by admitting small errors in classification and potentially using a more complex, *nonlinear decision boundary*, improving the generalization of the model.

15.1.1 Alternative Derivation

Consider a point $\mathbf{x}$. Let $\mathbf{d}$ be the vector from a hyperplane (*i.e.,* $\mathbf{w}\mathbf{x} + b = 0$) to $\mathbf{x}$ of minimum length. Let $\mathbf{x}_0$ be the projection of $\mathbf{x}$ onto the hyperplane. Then,

$$\mathbf{x}_0 = \mathbf{x} - \mathbf{d}.$$

As $\mathbf{d}$ is parallel to $\mathbf{w}$, so $\mathbf{d} = \alpha\mathbf{w}$ for some $\alpha \in \mathbb{R}$. Since $\mathbf{x}_0$ is on the hyperplane, $\mathbf{w}\mathbf{x}_0 + b = 0$. Thus,

$$\mathbf{w}\mathbf{x}_0 + b = \mathbf{w}(\mathbf{x} - \mathbf{d}) + b = \mathbf{w}(\mathbf{x} - \alpha\mathbf{w}) + b = 0.$$

Then, we get

$$\alpha = \frac{\mathbf{w}\mathbf{x} + b}{\mathbf{w}^T\mathbf{w}}.$$

The length of $\mathbf{d}$ is given by

$$\|\mathbf{d}\|_2 = \sqrt{\alpha^2\mathbf{w}^T\mathbf{w}} = \frac{|\mathbf{w}\mathbf{x} + b|}{\sqrt{\mathbf{w}^T\mathbf{w}}} = \frac{|\mathbf{w}\mathbf{x} + b|}{\|\mathbf{w}\|_2}.$$

We can obtain the margin by choosing the support vector, which is the closest point to the hyperplane by

$$\gamma(\mathbf{w}, b) = \min_{\mathbf{x}\in\mathcal{D}} \frac{|\mathbf{w}\mathbf{x} + b|}{\|\mathbf{w}\|_2}.$$

Note that the margin and hyperplane are scale invarianct:

$$\gamma(\beta\mathbf{w}, \beta b) = \gamma(\mathbf{w}, b).$$

15.2 Error Handling in SVM

In practice, it's unrealistic to expect a perfect separation of data, especially when the data is noisy or not linearly separable. To address this, we can **allow for some prediction errors while still striving to find an optimal decision boundary**.

One approach is to minimize the norm of the weight vector, while penalizing the number of errors N_e. The optimization problem can be formulated as follows:

$$\begin{aligned} &\min \frac{1}{2}\|\mathbf{w}\|^2 + C \cdot N_e, \text{ subject to} \\ &y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \quad \forall i. \end{aligned}$$

Here, C is a regularization parameter that controls the trade-off between minimizing the weight vector and the number of errors. The penalty approach described here is known as *0-1 loss*, where all errors are treated equally. However, this approach is not commonly used. Instead, a more practical approach introduces a *slack variable* with *hinge loss*. The slack variable (ξ_j) measures the degree of misclassification or how much a point is violating the margin. This leads to the following problem:

$$\begin{aligned} &\min \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_j \xi_j, \quad \text{subject to} \\ &\begin{cases} y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_j \ \forall i, \\ \xi_j \geq 0, \ \forall j. \end{cases} \end{aligned}$$

Note that $\xi_j > 1$, when SVMs make prediction errors:

$$\xi_j = (1 - (\mathbf{w}\mathbf{x}_j + b) \cdot y_j)$$

Let's look at the new constraint. If some data points are misclassified, then $\xi_j > 1$ and $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0$. This approach is called **soft-margin SVM**. Lastly, how do we set C? A large value of C places a higher penalty on errors, leading to a narrower margin but fewer misclassifications (*i.e.,* the SVM will try to classify all data points correctly), whereas a smaller value of C allows for a wider margin but potentially more misclassifications. The optimal value of C is typically chosen through cross-validation.

15.3 SVM Optimization: Lagrange Multipliers

15.3.1 Lagrange Multipliers

Consider the optimization problem:

$$\begin{aligned} &\min_{\mathbf{x}} f(\mathbf{x}) \\ &\text{subject to} \quad g(\mathbf{x}) = 0. \end{aligned}$$

To find the minimum of f under the constraint $g(\mathbf{x})$, we use the method of *Lagrange multipliers*. The key idea is that at the optimal point, the gradient of $f(\mathbf{x})$ must be parallel to the gradient of $g(\mathbf{x})$. Mathematically, this condition is expressed as:

$$\nabla f(\mathbf{x}) = \lambda \nabla g(\mathbf{x}).$$

Example: Consider a simple 2D example where you want to minimize the function $f(x, y) = x^2 + y^2$, which represents a circle centered at the origin. This function increases as you move away from the origin, so the minimum is at the origin.

Now, consider the constraint: $g(x, y) = x + y - 1 = 0$. This constraint is a line that runs through the xy-plane. Our goal is to find the point on this line that minimizes $f(x, y)$.

A Lagrange multiplier is like a balancing factor that adjusts the direction and magnitude of your search along the constraint. As you move along the constraint line $g(x, y)$, λ ensures that the solution also respects the shape of the function $f(x, y)$ that you are trying to minimize. To solve the constraint optimization problem, we define the Lagrangian function:

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda g(\mathbf{x}).$$

To find the minimum, we take the partial derivatives of $\mathcal{L}(\mathbf{x}, \lambda)$ with respect to both $\mathbf{x}$ and λ, and set them equal to zero.

15.3.2 SVM Optimization

Recall that we want to solve the following convex quadratic optimization problem:

$$\begin{aligned} &\min \frac{1}{2}\|\mathbf{w}\|^2, \quad \text{subject to} \\ &y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \quad \forall i. \end{aligned}$$

The objective is to find the optimal hyperplane that maximizes the margin between two classes of data points.

We can reformulate this optimization problem using the method of Lagrange multipliers, which introduces a set of multipliers α_i (*c.f.,* one for each constraint). The Lagrangian function for this problem is given by:

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1\right]$$

15.3.3 Duality and the Lagrangian Problem

While we could attempt to solve the primal optimization problem directly, it is often more practical, especially for large datasets, to reformulate the problem using the duality principle. The dual form is advantageous because it depends only on the inner products of the data points, which allows the use of *kernel* methods for non-linear classification.

To find the solution to the primal problem, we solve the following problem:

$$\max_{\mathbf{w},b} \min_{\alpha} \mathcal{L}(\mathbf{w}, b, \alpha)$$
$$\text{subject to} \quad \alpha_i \geq 0, \forall i.$$

Here, we maximize the Lagrangian with respect to the multipliers α_i, while minimizing with respect to the primal variables $\mathbf{w}$ and b.

15.3.4 Handling Inequality Constraints with KKT Conditions

You may observe that the method of Lagrange multipliers is used for equality constraints. However, it can be extended to handle inequality constraints through the use of additional conditions known as the **Karush-Kuhn-Tucker (KKT) conditions**. These conditions ensure that the solution satisfies the necessary optimality criteria for problems with inequality constraints. For more details on the KKT conditions.

15.4 The Wolfe Dual Problem

The Lagrangian problem for SVM optimization involves N inequality constraints, where N is the number of training examples. This problem is typically tackled by using its *dual form*. The duality principle provides a powerful framework, stating that **an optimization problem can be approached from two perspectives**:

1. The *primal problem*, which in our context is a minimization problem.
2. The *dual problem*, which is a maximization problem.

An important aspect of duality is that **the maximum value of the dual problem is always less than or equal to the minimum value of the primal problem.** This relationship means that the dual problem **provides a lower bound to the solution of the primal problem**.

In the context of SVM optimization, we are dealing with a convex optimization problem. According to *Slater's condition*, which applies to problems with affine constraints, strong duality holds. Strong duality implies that the optimal values of the primal and dual problems are equal, meaning the maximum value of the dual problem equals the minimum value of the primal problem. This equality allows us to solve the dual problem instead of the primal problem, often leading to computational advantages.

Recall that we aim to solve the following optimization problem:

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1\right]$$

The minimization problem involves solving the partial derivatives of $\mathcal{L}$ with respect to $\mathbf{w}$ and b and set them equal to zero:

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}, b, \alpha) = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i$$
$$\nabla_b \mathcal{L}(\mathbf{w}, b, \alpha) = -\sum_i \alpha_i y_i$$

Form the first equation, we obtain:

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

Next, we substitute the objective function with $\mathbf{w}$:

$$\begin{aligned}
\mathbf{W}(\alpha, b) &= \frac{1}{2}\left(\sum_i \alpha_i y_i \mathbf{x}_i\right) \cdot \left(\sum_j \alpha_j y_j \mathbf{x}_j\right) - \sum_i \alpha_i \left[y_i \left(\left(\sum_j \alpha_j y_j \mathbf{x}_j\right) \cdot \mathbf{x}_i + b\right) - 1\right] \\
&= \frac{1}{2}\Big(\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j\Big) - \sum_i \alpha_i \left[y_i \left(\Big(\sum_j \alpha_j y_j \mathbf{x}_j\Big) \cdot \mathbf{x}_i + b\right)\right] + \sum_i \alpha_i \\
&= \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_i \alpha_i y_i b + \sum_i \alpha_i \\
&= \sum_i \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j - \sum_i \alpha_i y_i b
\end{aligned}$$

Note that we use two indices, i and j when substituting $\mathbf{W}$. This is clear when we consider a simple example. Let's say you have two data points:

$$\mathbf{x}_1, y_1 = (1, 2), 1$$
$$\mathbf{x}_2, y_2 = (2, 1), 1$$

Then,

$$\|\mathbf{w}\|^2 = \mathbf{w} \cdot \mathbf{w} = \underbrace{(\alpha_1 y_1 \mathbf{x}_1 + \alpha_2 y_2 \mathbf{x}_2)}_{\sum_i} \cdot \underbrace{(\alpha_1 y_1 \mathbf{x}_1 + \alpha_2 y_2 \mathbf{x}_2)}_{\sum_j}.$$

This simplification shows that the optimization problem can be reformulated purely in terms of the Lagrange multipliers α_i. Note that the term involving b can be removed by setting $b = 0$, simplifying our equation further:

$$\mathbf{W}(\alpha, b) = \sum_i \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) \tag{15.1}$$

This expression is known as the **Wolfe dual Lagrangian function**. We have transformed the problem into one involving only the multipliers α_i, resulting in a quadratic programming problem, commonly referred to as the **Wolfe dual problem**:

$$\begin{aligned}
&\max_{\alpha} \mathbf{W}(\alpha, b) = \sum_i \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) \\
&\text{subject to } \alpha_i \geq 0 \text{ for any } i = 1, \ldots, m \\
&\sum_{i=1}^{m} \alpha_i y_i = 0
\end{aligned}$$

Once we get the value of α, the optimal $\mathbf{w}$ and b can be computed using

$$\alpha_i \left[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \right] = 0.$$

One important aspect of the dual problem is that it only involves the dot product of the input vectors $\mathbf{x}$. This property allows us to use of the *kernel trick* to handle non-linearly separable data by mapping it to a higher-dimensional space.

15.5 Karush-Kuhn-Tucker conditions

When dealing with optimization problems that involve inequality constraints, such as those encountered in Support Vector Machines (SVMs), an additional requirement must be met: the solution must satisfy the **Karush-Kuhn-Tucker (KKT) conditions**.

The KKT conditions are a set of first-order necessary conditions that must be satisfied for a solution to be optimal. These conditions extend the method of Lagrange multipliers to handle inequality constraints and are particularly useful in non-linear programming. For the KKT conditions to apply, the problem must also satisfy certain regularity conditions. Fortunately, one of these regularity conditions is *Slater*'s condition, which we have already established holds true for SVMs.

15.5.1 KKT Conditions and SVM Optimization

In the context of SVMs, the optimization problem is convex, meaning that the KKT conditions are not only necessary but also sufficient for optimality. This implies that if a solution satisfies the KKT conditions, it is guaranteed to be the optimal solution for both the primal and dual problems. Moreover, in this case, there is no duality gap, meaning the optimal values of the primal and dual problems are equal.

15.6 Prediction

Firstly, for a Linear SVM with no kernel, the primal weight vector is given by

$$w = \sum_{i \in \mathcal{S}} \alpha_i \, y_i \, x_i$$

Then, the decision function is

$$f(x) = w^\top x + b$$

Since the feature map $\phi(\,\cdot\,)$ may live in a huge or even infinite-dimensional space, we never form w explicitly. Instead we keep the *kernel trick* inside the decision function:

$$f(x) = \sum_{i \in \mathcal{S}} \alpha_i \, y_i \, K(x_i, \, x) + b,$$

where $K(x_i, x) = \langle \phi(x_i), \phi(x) \rangle$. Typical kernels are the RBF $K(u, v) = \exp\!\big(-\frac{\|u-v\|^2}{2\sigma^2}\big)$ or the polynomial $K(u, v) = (u^\top v + c)^p$.

Finally, we need to turn the decision value into a class label. For binary classification the prediction is simply the sign of the decision function:

$$\hat{y} = \text{sign}\big(f(x)\big) = \begin{cases} +1 & \text{if } f(x)0, \\ -1 & \text{if } f(x)0. \end{cases}$$

In sum,

$$\textbf{Predict}(x): \quad f(x) = \sum_{i \in \mathcal{S}} \alpha_i \, y_i \, K(x_i, x) + b, \; \hat{y} = \text{sign}\big(f(x)\big)$$

Chapter 16

Least Square SVM

16.1 Introduction

Least Squares Support Vector Machine (LS-SVM) is a modified version of the traditional Support Vector Machine (SVM) that simplifies the quadratic optimization problem by using a *least squares cost function*. LS-SVM transforms the quadratic programming problem in classical SVM into a set of linear equations, which are easier and faster to solve.

16.1.1 Optimization Problem (Primal Problem)

$$\min_{w,b,e} \frac{1}{2}\|w\|^2 + \frac{\gamma}{2}\sum_{i=1}^{N} e_i^2,$$
$$\text{subject to } y_i(w^T\phi(x_i) + b) = 1 - e_i,\ \forall i$$

where:

- w is the weight vector.
- b is the bias term.
- e_i are the error variables.

$$\begin{aligned}
\sum_{i=1}^{N} e_i^2 &= \sum_{i=1}^{N} \big(1 - y_i(w^T\phi(x_i) + b)\big)^2 \\
&= \sum_{i=1}^{N} \big(y_i^2 - y_i(w^T\phi(x_i) + b)\big)^2 \quad \text{, since } y_i = \pm 1,\ y_i^2 = 1 \\
&= \sum_{i=1}^{N} y_i^2 \big(y_i - (w^T\phi(x_i) + b)\big)^2 \\
&= \sum_{i=1}^{N} \big(y_i - (w^T\phi(x_i) + b)\big)^2
\end{aligned}$$

- γ is a regularization parameter.

- $\phi(x_i)$ is the feature mapping function.
- Note that $y_i^{-1} = y_i$, since $y_i = \pm 1$.

16.1.2 Lagrangian Function

To solve the constraint optimization problem, we define the Lagrangian function:

$$L(w, b, e, \alpha) = \min_{w,b,e} \frac{1}{2}\|w\|^2 + \frac{\gamma}{2}\sum_{i=1}^{N} e_i^2 - \sum_{i=1}^{n} \alpha_i \left[y_i(w^T\phi(x_i) + b) - 1 + e_i \right],$$

where α_i are Lagrange multipliers. Then, by setting the partial derivatives of the Lagrangian with respect to w, b, e, and α to zero, we get the KKT conditions.

- w:

$$\frac{\partial L}{\partial w} = w - \sum_{i=1}^{n} \alpha_i y_i \phi(x_i) = 0 \implies w = \sum_{i=1}^{n} \alpha_i y_i \phi(x_i)$$

- b:

$$\frac{\partial L}{\partial b} = -\sum_{i=1}^{n} \alpha_i y_i = 0$$

- e_i:

$$\frac{\partial L}{\partial e_i} = \gamma e_i - \alpha_i = 0 \implies \alpha_i = \gamma e_i$$

  Thus, $e_i = \frac{\alpha_i}{\gamma}$

- α_i:

$$\frac{\partial L}{\partial \alpha_i} = -\left[y_i(w^T\phi(x_i) + b) - 1 + e_i \right] = 0 \implies y_i(w^T\phi(x_i) + b) = 1 - e_i, i = 1, \ldots, N.$$

Let's substitute w and e:

- K: kernel matrix
- $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_n]^T$
- $y = [y_1, y_2, \ldots, y_n]^T$.
- $\Omega = YKY$, where $\Omega_{kl} = y_k y_l \phi(x_k)^T \phi(x_l)$
- $Y = \text{diag}(y)$.
- b: 1×1

Then, we can express it compactly

$$Y(KY^T\alpha + b\mathbf{1}) - \mathbf{1} + \frac{\alpha}{2\gamma} = 0$$
$$\mathbf{1}^T Y\alpha = 0$$

By using the expression of α and b, we get

$$\begin{bmatrix} 0 & y^T \\ y & \Omega + \frac{1}{\gamma}I \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{1} \end{bmatrix}$$

Note that the dimension of the matrix on the left-hand side is $(N+1) \times (N+1)$. Once we have b and α by solving the linear system, the decision function for **a new input** x can be obtained by:

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i K(x_i, x) + b.$$

Example: Suppose we have three training examples with feature vectors x_1, x_2, and x_3, and corresponding labels y_1, y_2, and y_3. The kernel matrix Ω is defined as:

$$\Omega_{ij} = y_i y_j K(x_i, x_j)$$

The dual form is:

$$\begin{bmatrix} 0 & y^T \\ y & \Omega + \frac{1}{\gamma}I \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{1} \end{bmatrix}$$

- $y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$
- $\alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$
- $e = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$
- I is a 3×3 identity matrix

Then, the Ω is given by

$$\Omega = \begin{bmatrix} y_1 y_1 K(x_1, x_1) & y_1 y_2 K(x_1, x_2) & y_1 y_3 K(x_1, x_3) \\ y_2 y_1 K(x_2, x_1) & y_2 y_2 K(x_2, x_2) & y_2 y_3 K(x_2, x_3) \\ y_3 y_1 K(x_3, x_1) & y_3 y_2 K(x_3, x_2) & y_3 y_3 K(x_3, x_3) \end{bmatrix}$$

Now, the complete matrix equation is:

$$\begin{bmatrix} 0 & y_1 & y_2 & y_3 \\ y_1 & \Omega_{11} + \frac{1}{\gamma} & \Omega_{12} & \Omega_{13} \\ y_2 & \Omega_{21} & \Omega_{22} + \frac{1}{\gamma} & \Omega_{23} \\ y_3 & \Omega_{31} & \Omega_{32} & \Omega_{33} + \frac{1}{\gamma} \end{bmatrix} \begin{bmatrix} b \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

This can be written explicitly as:

$$\begin{bmatrix} 0 & y_1 & y_2 & y_3 \\ y_1 & y_1^2 K(x_1, x_1) + \frac{1}{\gamma} & y_1 y_2 K(x_1, x_2) & y_1 y_3 K(x_1, x_3) \\ y_2 & y_2 y_1 K(x_2, x_1) & y_2^2 K(x_2, x_2) + \frac{1}{\gamma} & y_2 y_3 K(x_2, x_3) \\ y_3 & y_3 y_1 K(x_3, x_1) & y_3 y_2 K(x_3, x_2) & y_3^2 K(x_3, x_3) + \frac{1}{\gamma} \end{bmatrix} \begin{bmatrix} b \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

The solution to this matrix equation provides the values of b and $\alpha_1, \alpha_2, \alpha_3$, which are then used to construct the decision function:

$$f(x) = \sum_{i=1}^{3} \alpha_i y_i K(x, x_i) + b$$

16.2 LS-SVM with Asymmetric Kernels

Recall that the dual form of LS-SVM is given by

$$\begin{bmatrix} 0 & y^T \\ y & \Omega + \frac{1}{\gamma} I \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ e \end{bmatrix}$$

An interesting point here is that using an asymmetric kernel in LS-SVM will not reduce to its symmetrization and asymmetric information can be learned. Then we can develop asymmetric kernels in the LS-SVM framework in a straightforward way.

Asymmetric kernels are particularly useful in capturing directional relationships in data that symmetric kernels cannot. For instance, in scenarios involving directed graphs or conditional probabilities, the relationship from x to y is inherently different from the relationship from y to x.

16.2.1 AsK-LS Primal Problem Formulation

We first define a generalized kernel trick for an inner product of two mappings ϕ_s and ϕ_t.

$$K(\mathbf{u}, \mathbf{v}) = \langle \phi_s(\mathbf{u}), \phi_t(\mathbf{v}) \rangle, \forall \mathbf{u} \in \mathbb{R}^{d_s}, \mathbf{v} \in \mathbb{R}^{d_t},$$

where $\phi_s : \mathbb{R}^{d_s} \to \mathbb{R}^p$, $\phi_t : \mathbb{R}^{d_t} \to \mathbb{R}^p$, and $\mathbb{R}^p$ is a high-dimensional or even an infinite-dimensional space. Note that d_s and d_t can be different.

The primal problem for AsK-LS is formulated to handle these asymmetric relationships. The goal is to find the weight vectors ω and ν, and bias terms b_1 and b_2, that minimize the following objective function:

$$\min_{\omega,\nu,b_1,b_2,e,h} \frac{1}{2}\omega^T\nu + \frac{\gamma}{2}\sum_{i=1}^{m} e_i^2 + \frac{\gamma}{2}\sum_{i=1}^{m} h_i^2,$$

subject to the constraints:

$$y_i(\omega^T \phi_s(x_i) + b_1) = 1 - e_i$$
$$y_i(\nu^T \phi_t(x_i) + b_2) = 1 - h_i$$

Here:

- ω and ν are weight vectors for the source and target features.
- $\phi_s(x)$ and $\phi_t(x)$ are the source and target feature mappings.
- e_i and h_i are error terms for the source and target constraints.
- γ is a regularization parameter.

Note that this formulation is almost the same as the LS-SVM except that this considers both the source and target feature spaces simultaneously.

16.2.2 Dual Form

Let's transform it into a *dual* form. The dual problem involves solving a system of linear equations derived from the primal problem's Lagrangian. The Lagrangian function for the primal problem is:

$$\mathcal{L}(\omega, \nu, b_1, b_2, e, h, \alpha, \beta) =$$
$$\frac{1}{2}\omega^T\nu + \frac{\gamma}{2}\sum_{i=1}^{m} e_i^2 + \frac{\gamma}{2}\sum_{i=1}^{m} h_i^2 +$$
$$\sum_{i=1}^{m} \alpha_i(1 - e_i - y_i(\omega^T\phi_s(x_i) + b_1)) + \sum_{i=1}^{m} \beta_i(1 - h_i - y_i(\nu^T\phi_t(x_i) + b_2))$$

The KKT conditions are derived by setting the partial derivatives of the Lagrangian with respect to ω, ν, b_1, b_2, e, and h to zero. The dual problem leads to the following linear system:

$$\begin{bmatrix} 0 & 0 & Y^T & 0 \\ 0 & 0 & 0 & Y^T \\ Y & 0 & \frac{I}{\gamma} & H \\ 0 & Y & H^T & \frac{I}{\gamma} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

where:

- Y is a vector of class labels.
- H is the kernel matrix with elements $H_{ij} = y_i K(x_i, x_j) y_j$, where $K(x_i, x_j) = \langle \phi_s(x_i), \phi_t(x_j) \rangle$ is the asymmetric kernel function.
  - For an asymmetric kernel K, the kernel function $K(x_i, x_j) \neq K(x_j, x_i)$. This asymmetry is directly incorporated into the matrix H, where:

$$H_{ij} = y_i K(x_i, x_j) y_j$$
$$H_{ji} = y_j K(x_j, x_i) y_i$$

AsK-LS uses two different feature mappings ϕ_s and ϕ_t for the source and target features. This approach allows capturing more information compared to symmetric kernels. The dual solution provides weight vectors ω and ν, which span the target and source feature spaces, respectively.

The decision functions for classification from the source and target perspectives are given by

$$f_t(x) = \sum_{i=1}^{m} \alpha_i y_i K(x_i, x) + b_1$$
$$f_s(x) = \sum_{i=1}^{m} \beta_i y_i K(x, x_i) + b_2$$

These functions utilize the learned asymmetric relationships in the data.

16.2.3 Asymmetric Kernels

We can consider asymmetric kernels like these:

$$K_{SNE}(\mathbf{x}, \mathbf{y}) = \frac{\exp(-\|\mathbf{x} - \mathbf{y}\|_2^2)/\sigma^2}{\sum_{\mathbf{z} \in \mathbf{X}_{train}} \exp(-\|\mathbf{x} - \mathbf{z}\|_2^2)/\sigma^2}$$

$$K_T(\mathbf{x}, \mathbf{y}) = \frac{(1 + \|\mathbf{x} - \mathbf{y}\|_2^2)^{-1}}{\sum_{\mathbf{z} \in \mathbf{X}_{train}} (1 + \|\mathbf{x} - \mathbf{z}\|_2^2)^{-1}}$$

Part IV

Generative Modeling

Chapter 17

Introduction

17.1 KL Divergence

The KL divergence can be defined as follows:

$$D_{KL}(P||Q) = \mathbb{E}_{x\sim P}\left[\log \frac{P(X)}{Q(X)}\right]$$

17.1.1 Properties

- Non symmetric
- $D_{KL} \in [0, \infty]$
- In order for the KL divergence to be finite, the support of P needs to be in the support of Q.

17.1.2 Rewriting the Objective

$$\begin{aligned} D_{KL}(P||Q) &= \mathbb{E}_{x\sim P}\left[\log \frac{P(X)}{Q(X)}\right] \\ &= \mathbb{E}_{x\sim P}[-\log Q(X)] - \mathcal{H}(P(X)) \end{aligned}$$

- $\mathbb{E}_{x\sim P}[-\log Q(X)]$: Cross entropy
- $\mathcal{H}(P(X))$: Entropy of P

17.1.3 Forward and Reverse KL

Let's say there is a true distribution $P(X)$ with two modes and our approximation $Q(X)$ has one mode. Then,

- Forward KL: $D_{KL}(P||Q)$
- Reverse KL: $D_{KL}(Q||P)$

Forward KL: Mean-Seeking Behavior

$$\begin{aligned}\arg\min_\theta D_{KL}(P\|Q) &= \arg\min_\theta \mathbb{E}_{x\sim P}[-\log Q_\theta(X)] - \mathcal{H}(P(X)) \\ &= \arg\min_\theta \mathbb{E}_{x\sim P}[-\log Q_\theta(X)] \\ &= \arg\max_\theta \mathbb{E}_{x\sim P}[\log Q_\theta(X)]\end{aligned}$$

Intuition: x will be sampled from the distribution P, and its value will be estimated from Q. Thus, there will be higher chance that x will be sampled from a space with higher probablity in P. Therefore, Q_θ has to consider all modes, which have high probabilities.

To use the forward KL, we have to have an access to the true model $P(X)$ for sampling.

Reverse KL: Mode-Seeking Behavior

$$\begin{aligned}\arg\min_\theta D_{KL}(Q\|P) &= \arg\min_\theta \mathbb{E}_{x\sim Q_\theta}[-\log P(X)] - \mathcal{H}(Q_\theta(X)) \\ &= \arg\max_\theta \mathbb{E}_{x\sim Q_\theta}[\log P(X)] + \mathcal{H}(Q_\theta(X))\end{aligned}$$

Intuition: x will be sampled from the distribution Q, and its value will be estimated from P. Thus, there will be higher chance that x will be sampled from a space with higher probablity in Q. Therefore, to maximize the value, we need to focus on a single mode.

To use the reverse KL, we have to be able to evaluate the true model $P(X)$.

Chapter 18

Sampling Based Inference

18.1 Basic Sampling Methods

18.1.1 Inverse Transform Sampling

Inverse transform sampling is a basic method for pseudo-random number sampling, *i.e.,* for generating sample numbers at random from any probability distribution given its cumulative distribution function (CDF).

Assume that we already have a uniformly distributed random number generator, *e.g.,* np.random.randn()

1. Generate a random number $u \sim Unif[0, 1]$
2. Find the inverse of the desired CDF, $F_X^{-1}(x)$.
3. Compute $X = F_X^{-1}(u)$. The computed random variable X has distribution $F_X(x)$

However, it is **hard to compute the inverse of CDF** ($F_X(x)$)

- $F_X(x) : \mathbb{R} \mapsto [0, 1]$ is any CDF.
- CDF is a non-negative and non-decreasing (monotone) function that is continuous.
- Our objective is to simulate a random variable X distributed as F; that is, we want to simularte a X such that $P(X \leq x) = F(x)$.
- F is invertible since it is continuous and strictly increasing.

18.1.2 Ancestral Sampling

$$p(\mathbf{x}) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_2)\cdots$$

Sampling steps:

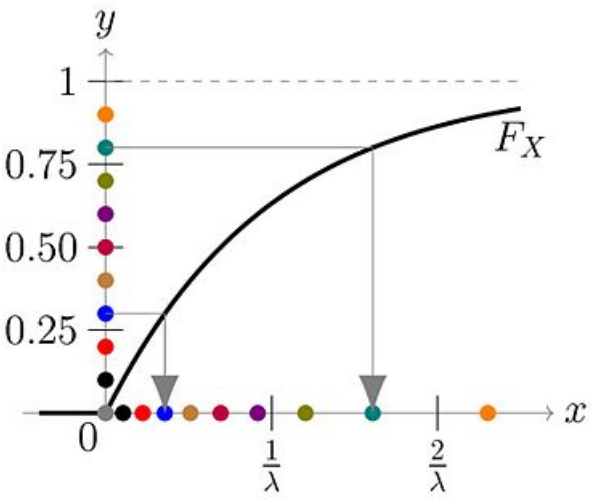


Figure 18.1: y-axis: Uniform distribution, x-axis: sample value

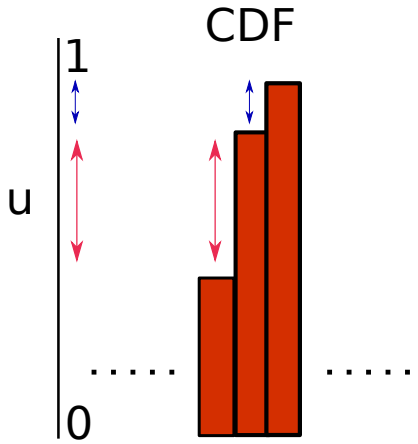


Figure 18.2: How can this sampling method recover the original distribution?

1. sample $\mathbf{x}_1$
2. sample $\mathbf{x}_2$ conditioned by $\mathbf{x}_1$
3. sample $\mathbf{x}_3$ conditioned by $\mathbf{x}_2$

18.1.3 Rejection Sampling

Rejection sampling is a simple method. It rejects samples violating a given condition (*e.g.,* conditions of conditional probability.). Let's see its theory.

Rejection sampling is a method for sampling from a distribution $p(x) = \frac{1}{Z}p'(x)$ that is difficulut to sample directly, but its unnormalized pdf $p'(x)$ is east to evaluate (Z is hard to compute). In rejection sampling, we need some simpler distribution $q(x)$, called a **proposal distribution**.

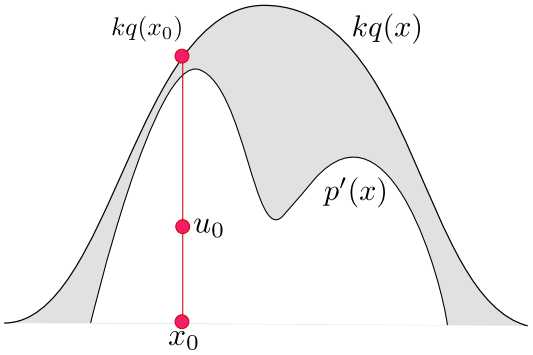
The intuition of rejection sampling is actually similar to Monte-Carlo estimation. By setting a large area (proposal distribution), we can sample points and take them that are inside the our

target distribution

To run the rejection sampling, introduce a constant k whose value is chosen such that $kq(x) \geq p'(x)$ for all values of x. The function $kq(x)$ is called a comparison function. Each step of the rejection sampler involves generating two random variables:

1. Sample $x_0 \sim q$
2. Sample $u_0 \sim U[0, kq(x_0)]$.

Finally, If $u_0 > p'(x_0)$, then the sample x_0 will be rejected, otherwise we add the sample x_0 to our set of samples $\{x^r\}$.



The original values of x are generated from the distribution $q(x)$ and these samples are then accepted with probability $p'(x)/kq(x)$ (see the figure above. The acceptance probability (*i.e.,* length) is the p' divided by kq). Then, the probability that a sample will be accepted is given by

$$\begin{aligned} p(accept) &= p\left(u \leq \frac{p'(x)}{kq(x)}\right) \\ &= \int p\left(u \leq \frac{p'(x)}{kq(x)}\middle| x\right) q(x)dx \\ &= \int \frac{p'(x)}{kq(x)} q(x)dx \\ &= \frac{1}{k}\int p'(x)dx \end{aligned}$$

Thus, the sampling will be more efficient if we choose small k to increase the change of acceptance.

18.1.4 Importance Sampling

We want to estimate an expectation of function $f(x)$, where $x \sim p(x)$, but it is hard to estimate the distribution $p(x)$. Again, the importance sampling is not a method for generating samples from $p(\mathbf{x})$. In this case, we can use a simple distribution $q(x)$ by

$$\begin{aligned}\mathbb{E}_p[f(\mathbf{x})] &= \int p(\mathbf{x})f(\mathbf{x})d\mathbf{x} \\ &= \int p(\mathbf{x})f(\mathbf{x})\frac{q(\mathbf{x})}{q(\mathbf{x})}d\mathbf{x} \\ &= \int q(\mathbf{x})\left[f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}\right]d\mathbf{x} \\ &= \mathbb{E}_q\left[f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}\right]\end{aligned}$$

- Assume that $p(\mathbf{x})$ is known and too complicated to be sampled directly.
- Samples are independently drawn from a **proposal density** $Q(\mathbf{x})$, which is designed to be close to the true density $p(\mathbf{x})$ and **simpler**
- Generate R samples from $Q(\mathbf{x})$

By applying the Monte-Carlo method, we can get

$$\mathbb{E}_q\left[f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}\right] \approx \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}, \quad \mathbf{x}_i \sim p(\mathbf{x}) \tag{18.1}$$

- Unbiased estimation
- (Potentially) Smaller variance compared to the vanilla Monte-Carlo method above.
  - $Var_q\left[f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}\right] < Var_p[f(\mathbf{x})]$
  - When $q(\mathbf{x})$ is high where $|p(\mathbf{x})f(\mathbf{x})|$ is high.

Chapter 19

Markov Chain Monte Carlo

19.1 Gibbs Sampling

The phrase "Markov chain Monte Carlo" encompasses a broad array of techniques that have in common a few key ideas. The setup for all the techniques that we will discuss in this book is as follows:

1. We want to sample from a some complicated density or probability mass function π. Often, this density is the result of a Bayesian computation so it can be interpreted as a posterior density. The presumption here is that we can evaluate π but we cannot sample from it.
2. We know that certain stochastic processes called Markov chains will converge to a stationary distribution (if it exists and if specific conditions are satisfied). Simulating from such a Markov chain for a long enough time will eventually give us a sample from the chain's stationary distribution.
3. Given the functional form of the density π, we want to construct a Markov chain that has π as its stationary distribution.
4. We want to sample values from the Markov chain such that the sequence of values $\{x_n\}$ generated by the chain converges in distribution to the density π.

In order for all these ideas to make sense, we need to first go through some background on Markov chains. The rest of this chapter will be spent defining all these terms, the conditions under which they make sense, and giving examples of how they can be implemented in practice.

19.2 Markov Chain

Reference Link

A Markov chain is a stochastic process that evolves over time by transitioning into different states. The sequence of states is denoted by the collection $\{X_i\}$ and the transition between states is random. Formally,

Definition 1 *Let D be a finite set. A random process $X_1, X_2, \ldots$ with values in D is called a Markov chain if*

$$P(X_t = x_{t+1} | X_t = x_t, \ldots, X_0 = x_0) = P(X_{t+1} = x_{t+1} | X_t = x_t)$$

We can think of X_t as a random state at time t, and the Markovian assumption is that the probability of transitioning from x_t to x_{t+1} only depends on x_t. In other words, the future state depends only on the present. Let p_{ij} be the probability of transitioning from state i to state j. A Markov chain can be defined by a transition probability matrix:

Definition 2 *The matrix $\mathbf{P} = (p_{ij})_{i,j} \in D$ is called the transition probability matrix.*

Thus, P is a $D \times D$ matrix, where $|D|$ denotes the cardinality of D, and the cell value p_{ij} is the probability of transitioning from state i to state j, and the rows of P must sum to one. We will restrict ourselves to time *homogeneous Markov chains*:

Definition 3 *A Markov chain is called time homogeneous if*

$$\mathbb{P}\{X_{t+1} = j \,|\, X_n = i\} = p_{ij}, \, \forall n.$$

It state that *the transition probabilities are not changing as a function of time.* Finally, let's introduce some useful notation for the initial state of the Markov chain. Let

$$\mathbb{P}_{x_0}\{\cdot\} \triangleq \mathbb{P}\{\cdot | X_0 = x_0\}.$$

For example, I will write $\mathbb{P}_a\{X_1 = b\}$ rather than $\mathbb{P}\{X_1 = b | X_0 = a\}$ for simplicity.

Consider a simple Markov chain modeling the weather. The weather has two states: rainy and sunny. Thus, $D = \{r, s\}$ and X_n is the "weather on day n". The Markov chain model is as follows. If today is rainy (r), tomorrow it is sunny (s) with probability p. If today it is sunny, tomorrow it is rainy with probability q. Then, transition matrix is given by

$$\mathbf{P} = \begin{bmatrix} 1-p & p \\ q & 1-q \end{bmatrix}.$$

The state diagram of the chain can be represented as follows: As a consequence of the Markovian

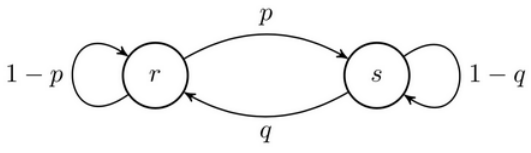


Figure 19.1: A sample Markov chain.

assumptions, the probability of any path on a Markov chain is just the multiplication of the numbers along the path. For example, for some Markov chain with states $D = \{a, b, c, d\}$, the probability of a particular path, say $a \to b \to b \to d \to c$ factorize as

$$p_{ab} \cdots p_{dc}$$

Let's try to formulate this by

$$\mathbb{P}_i\{X_n = j\}.$$

For instance, let's say $n = 2$. Then, we have

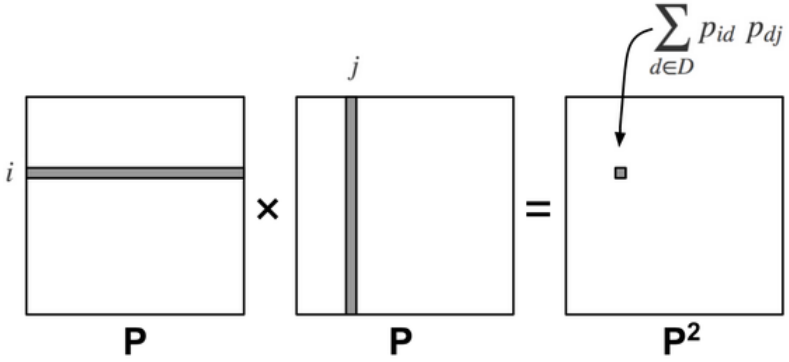
$$\begin{aligned}\mathbb{P}_i\{X_2 = j\} &= \sum_{d\in D} \mathbb{P}_i\{X_2 = j, X_1 = d\} \\ &= \sum_{d\in D} \mathbb{P}_i\{X_2 = j | X_1 = d\}\mathbb{P}_i\{X_1 = d\} \\ &= \sum_{d\in D} p_{id}p_{dj}\end{aligned}$$

This is equivalent to a dot product of the i-th row to j-th column of the transition matrix $\mathbb{P}$. This can be expressed as follows:

$$\mathbb{P}\{X_2 = j | X_0 = i\} = \sum_{d\in D} p_{id}p_{dj} = \left(\mathbf{P}^2_{ij}\right).$$

This can be generalized to

$$\mathbb{P}_i\{X_n = j\} = \left(\mathbf{P}^n_{ij}\right).$$



In sum, the dot product performs marginalization, and everything works out nicely thanks to the Markovian assumption. If the D-dimensional vector v represents a discrete distribution over initial states X_0, then $\mathbf{v^T P}$ is a D-dimensional vector representing the probability distribution over X_1.

19.2.1 Ergodicity

Let's discuss about *ergodicity*, which is a property of a random process in which its time average is the same as its probability space average. It can be defined as follows:

Definition 4 *A Markov chain $\{X_n\}$ is called ergodic if the limit*

$$\boldsymbol{\pi}(j) = \lim_{n\to\infty} \mathbb{P}_i\{X_n = j\}$$

exists for every state j and does not depend on the initial state i. The D-dimensional vector $\boldsymbol{\pi}(j)$ is called the stationary probability.

In other words,

- The probability $\boldsymbol{\pi}(j)$ of reaching at state j (*i.e.,* $\mathbb{P}_i\{X_n = j\}$)
- After a long time (*i.e.,* $\lim_{n\to\infty}$)
- Regardless of the initial state i (*i.e.,* $\mathbb{P}_i\{X_n = j\}$).

Equivalently, it can be expressed as

$$\boldsymbol{\pi}(j) = \lim_{n\to\infty} \left(\mathbf{P}^n\right)_{ij}.$$

The ergodicity gives the following property:

$$\begin{aligned}
\boldsymbol{\pi}(j) &= \lim_{n\to\infty} \left(\mathbf{P}^n\right)_{ij} \\
&\overset{\star}{=} \lim_{n\to\infty} \left(\mathbf{P}^{n+1}\right)_{ij} \\
&= \lim_{n\to\infty} \left(\mathbf{P}^n\mathbf{P}\right)_{ij} \\
&= \lim_{n\to\infty} \sum_{d\in D} \left(\mathbf{P}^n\right)_{id} \mathbf{P}_{dj} \\
&= \sum_{d\in D} \boldsymbol{\pi}(d)\mathbf{P}_{dj}
\end{aligned}$$

- The step $\star$ holds since the step n and $n+1$ does not matter under the limit.

Finally, we can write this as

$$\boldsymbol{\pi}^T = \boldsymbol{\pi}^T\mathbf{P},$$

where $\boldsymbol{\pi}$ is a column vector. Hence, the name "stationary probability distribution" denotes that it is a distribution that does not change over time. Note that it can be also written as:

$$\mathbf{P}^T\boldsymbol{\pi} = \boldsymbol{\pi}.$$

Then, we can say $\boldsymbol{\pi}$ is an eigenvector of $\mathbf{P}^T$ with eigenvalue of 1. Thus, we can obtain the stationary distribution $\boldsymbol{\pi}$ from an eigenvectors and eigenvalues of $\mathbf{P}^T$.

Since we are interested in ergodicity, let's now introduce some properties related to reachability and long-term behavior.

Definition 5 *We say that there is a path from i to j ($i \rightsquigarrow j$) if there is a nonzero probability that starting at i, we can reach j at some point in the future.*

Definition 6 *A state i is called **transient** if there exists a state j such that $i \rightsquigarrow j$ but $j \not\rightsquigarrow i$.*

Definition 7 *A state i is called **recurrent** if for all states j there exist $i \rightsquigarrow j$ and $j \rightsquigarrow i$.*

Definition 8 *A Markov chain is **irreducible** if $i \leftrightarrow j, \forall i, j \in S$. Simply, if all states are able to visit other states, it is irreducible.*

Definition 9 *State i has a **period** d (*i.e., *periodically visit the state i) $\leftrightarrow$ aperiodic.*

Intuitively, a *transient* state is a state that cannot return to itself; while a *recurrent* state can return. In other words, these two conditions are opposite. A transient state is not recurrent, and a recurrent state is not transient. Note that if a state is recurrent, every reachable state is also recurrent. We think of a set of recurrent states as a "class" or a "recurrent class". We can notice

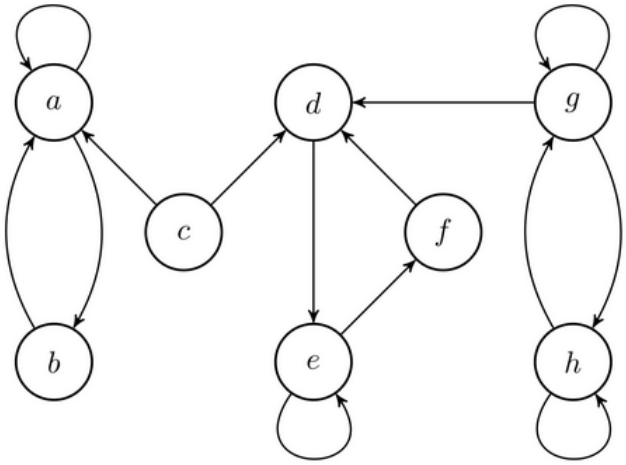


Figure 19.2: A Markov chain with $D = \{a, b, c, d, e, f, g, h\}$. The state c is a transient state. Note that g and h are also transient as there exist states that they cannot return. There are two recurrent classes: $\{a, b\}$ and $\{d, e, f\}$.

that Fig. 19.1 is ergodic but Fig. 19.2 is not since some states are not recurrent.

In sum a state is ergodic if the state is recurrent and aperiodic. Markov chain is ergodic if all states are ergodic.

19.2.2 Limit Theorem of Markov chain

Reference Link

For a Markov chain with a discrete state space and transition matrix P, let π_* be such that $\pi_* P = \pi_*$. Then π_* is a stationary distribution of the Markov chain and the chain is said to be stationary if it reaches this distribution.

The basic limit theorem for Markov chains says that, under a specific set of assumptions that we will detail below, we have

$$||\pi_* - \pi_n|| \to 0$$

as $n \to \infty$, where $||\cdot||$ is the total variation distance between the two densities. Therefore, no matter where we start the Markov chain (π_0), π_n will eventually approach the stationary distribution. Another way to think of this is that

$$\lim_{n\to\infty} \pi_n(i) = \pi_*(i).$$

for all states i in the state space. Note that π_0 is the probability distribution of the Markov chain at time 0. Also, π_n denote the distribution of the chain at time n.

19.2.3 Time Reversibility

Consider a stationary ergodic Markov chain with transition probability $p(i, j)$ and stationary distribution $\pi(i)$, if we reverse the process, we will get a reversed Markov chain with transition probability $q(i, j)$:

$$\begin{aligned} q(j,i) &= P(X_m = i | X_{m+1} = j) \\ &= \frac{P(X_m = i, X_{m+1} = j)}{P(X_{m+1} = j)} \\ &= \frac{P(X_m = i | X_{m+1} = j) P(X_{m+1} = j)}{P(X_{m+1} = j)} \\ &= \frac{\pi(i) p(i,j)}{\pi(j)} \\ \pi(i) p(i,j) &= \pi(j) q(j,i) \end{aligned}$$

If $p(i, j) = q(j, i)$, it is called time-reversible Markov chain.

19.3 Markov Chain Monte Carlo

MCMC aims to generate samples from some complex probability distribution $p(x)$ that is difficult to directly sample from.

The basic sampling methods we have learnt so far do not leverage past information, which assumes all samples are independent. In Markov chain based sampling, we will treat random variables as a sequence of sampling process.

In Markov Chain Monte Carlo(MCMC), we assume that a stationary distribution is already known. We are more interested in estimating a transition rule that describing the stationary distribution.

Ground rules for MCMCs:

- MCMCs stochastically explore the parameter space in such a way that the histogram of their samples produces the target distribution.
- Markovian: Evolution of the chain (*i.e.,* collections of samples from one iteration to the other) only depends on the current position and some transition probability distribution (*i.e.,* how we move from one point in parameter space to another). This means that the chain has no memory and past samples cannot be used to determine new positions in parameter space.
- The chain will converge to the target distribution if the transition probability is:
  - Irreducible: From any point in parameter space, we must be able to reach any other point in the space in a finite number of steps.
  - Positive recurrent: For any point in parameter space, the expected number of steps for the chain to return to that point is finite. This means that the chain must be able to re-visit previously explored areas of parameter space.
  - Aperiodic: The number of steps to return to a given point must not be a multiple of some value k. This means that the chain cannot get caught in cycles.

19.3.1 Metropolis-Hasting Algorithm

Suppose we have a target posterior distribution $\pi(x)$, where x here can be any collection of parameters (not a single parameter). In order to move around this parameter space we must formulate some proposal distribution:

$$q(x_{i+1} \mid x_i),$$

that specifies the probability of moving to a point in parameter space, x_{i+1}, given that we are currently at x_i. The Metropolis Hastings algorithm accepts a "jump" to x_{i+1} with the following probability

$$\kappa(x_{i+1} \mid x_i) = \min\left(1, \frac{\pi(x_{i+1})q(x_i \mid x_{i+1})}{\pi(x_i)q(x_{i+1} \mid x_i)}\right) = \min(1, H),$$

where the fraction above is called the Hastings ratio, H. The above expression represents that the probability of transitioning from point x_{i+1} given the current position x_i is a function of the ratio of the value of the posterior at the new point to the old point (*i.e.*, $\pi(x_{i+1})/\pi(x_i)$) and the ratio of the transition probabilities at the new point to the old point (*i.e.*, $q(x_i \mid x_{i+1})/q(x_{i+1} \mid x_i)$). Firstly, it is clear that if the ratio is bigger than 1 then the jump will be accepted. Secondly, the ratio of the target posteriors ensures that the chain will gradually move to high probability regions. Lastly, the ratio of the transition probabilities ensures that the chain is not "favored" toward certain locations by the proposal distribution function. Note that many proposal distributions are symmetric (*i.e.*, $q(x_{i+1} \mid x_i) = q(x_i \mid x_{i+1})$).

The Metropolis-Hasting algorithm is then:

```
def mh_sampler(x0, lnprob_fn, prop_fn, prop_fn_kwargs={}, iterations=100000):
    """Simple metropolis hastings sampler.

    :param x0: Initial array of parameters.
    :param lnprob_fn: Function to compute log-posterior.
    :param prop_fn: Function to perform jumps.
    :param prop_fn_kwargs: Keyword arguments for proposal function
    :param iterations: Number of iterations to run sampler. Default=100000

    :returns:
        (chain, acceptance, lnprob) tuple of parameter chain , acceptance rate
        and log-posterior chain.
    """

    # number of dimensions
    ndim = len(x0)

    # initialize chain, acceptance rate and lnprob
    chain = np.zeros((iterations, ndim))
    lnprob = np.zeros(iterations)
    accept_rate = np.zeros(iterations)

    # first samples
    chain[0] = x0
    lnprob0 = lnprob_fn(x0)
    lnprob[0] = lnprob0

    # start loop
    naccept = 0
    for ii in range(1, iterations):

        # propose
        x_star, factor = prop_fn(x0, **prop_fn_kwargs)

        # draw random uniform number
        u = np.random.uniform(0, 1)

        # compute hastings ratio
        lnprob_star = lnprob_fn(x_star)
        H = np.exp(lnprob_star - lnprob0) * factor

        # accept/reject step (update acceptance counter)
        if u < H:
            x0 = x_star
            lnprob0 = lnprob_star
            naccept += 1

        # update chain
        chain[ii] = x0
        lnprob[ii] = lnprob0
```

```
51          accept_rate[ii] = naccept / ii
52
53      return chain, accept_rate, lnprob
```

Chapter 20

Topic Modeling

20.1 Latent Semantic Allocation

Topic model provides insights like

- Can analyze topics. *e.g.*,, a certain topic includes specific words more than other topics.
- A certain document's topic distribution (simplex)

pLSA: Latent Variable Model

$$P_{LSA}(w|d) = \sum_z P(w|z;\theta)P(z|d;\pi)$$

- w: word
- d: document
- z: latent variable

Equivalently,

$$P_{LSA}(d,w) = \sum_z P(w|z)P(d|z)p(z) = p(d)\sum_z P(w|z)P(z|d)$$

The probability of observing $n(w_i, d_j)$ occurrences of word w_i in document d_j is given by

$$p(w_i, d_j)^{n(w_i,d_j)}$$

The probability of observing the complete document collection is then given by the product of probabilities of observing every single word in every document with corresponding number of occurrences.

Then, the likelihood function becomes

$$L = \prod_{i=1}^{m} \prod_{j=1}^{n} p(w_i, d_j)^n(w_i, d_j)$$

The log-likelihood is then

$$\begin{aligned}\mathcal{L} &= \sum_{i=1}^{m} \sum_{j=1}^{n} n(w_i, d_j) \log(p(w_i, d_j)) \\ &= \sum_{l=1}^{k} p(w_i|z_l)p(d_j|z_l)p(z_l)\end{aligned}$$

Parameter Inference:

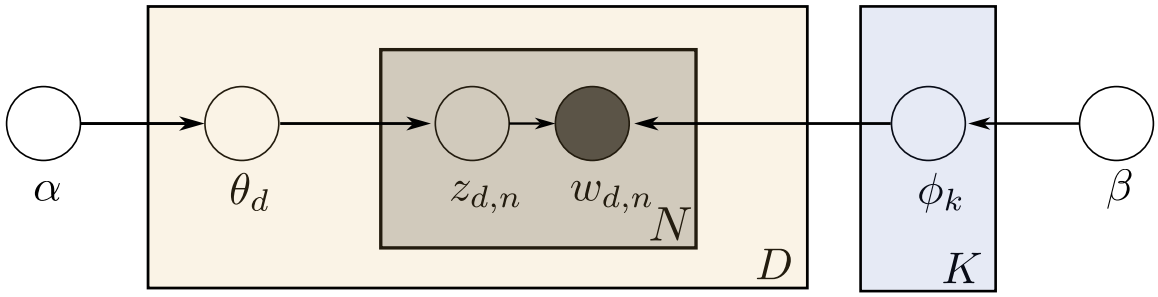
- We cannot maximize the likelihood analytically because of the logarithm of the sum
- A standard procedure is to use *EM*.

20.2 Latent Dirichlet Allocation

The assumptions of LDA:

- Each topic is a distribution over words.
- Each document is a mixture of corpus-wide topics.
- Each word is sampled from one of topics.

The LDA attempts to model the document generation process stochastically. However, we have to infer the latent structure (the distributions) of documents.



- $\theta_d \sim Dir(\alpha)$: For each document, draw topic distribution.
  - α: Dirichlet parameter
- $z_{d,n} \sim Mult(\theta_d)$: per-word topic assignment. The n-th word of document d is from which topic?
- $w_{d,n} \sim Mult(\phi_{z_{d,n}}, n)$: observed word. The n-th word in a document d is from a certain topic ($z_{d,n}$) distribution $\phi_{z_{d,n}}$.

- $\phi_k \sim Dir(\beta), i = \{1, \ldots, K\}$: topics.
  - β: topic hyperparameter (Dirichlet parameter).

We can immediately notice that the LDA's modeling approach is quite far from the way we write texts. However, LDA works quite well.

The document generation process can be modelled as follows:

$$p(\phi_{1:K}, \theta_{1:D}, z_{1:D}, w_{1:D}) = \prod_{i=1}^{K} p(\phi_i|\beta) \prod_{d=1}^{D} p(\theta_d|\alpha) \left(\prod_{n=1}^{N} p(w_{d,n}|\phi_{1:K}, z_{d,n}) p(z_{d,n}|\theta_d) \right).$$

20.2.1 LDA Inference

The posterior of the latent variables given the document is

$$p(\phi, \theta, \mathbf{z}|\mathbf{w}) = \frac{p(\phi, \theta, \mathbf{z}, \mathbf{w})}{\int_\phi \int_\theta \sum_{\mathbf{z}} p(\phi, \theta, \mathbf{z}, \mathbf{w})}$$

Computing the posterior is intractable:

- The denominator is intractable
- We cannot compute the denominator, the marginal p(w).
- We are going to use collapsed Gibbs sampling.

We want to estimate the topic distribution **z**.

20.2.2 Dirichlet Distribution

The Dirichlet Distribution can be considered as a extension of the *beta distribution*.

$$p(P = \{p_i\}|\alpha_i) = \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i p_i^{\alpha_i - 1} \tag{20.1}$$

- $\sum_i p_i = 1$
- The posterior distribution of Dirichlet distribution is also Dirichlet distribution.

Chapter 21

Latent Variable Models

21.1 Motivation of Latent Variable Models

Let's say we want to classify some data. If we had access to a corresponding latent variable for each observation $\mathbf{x}_i$, modeling would be more straightforward. To illustrate this, consider the challenge of finding the latent variable (*i.e.,* the true class of $\mathbf{x}$) $z^* = \text{argmax}_z\, p(\mathbf{x}|z)$, as shown in Fig. 21.1(b).

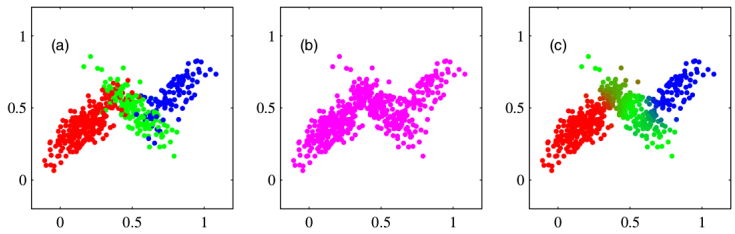


Figure 21.1: (a) Complete dataset $p(\mathbf{x}|z)$. (b) Incomplete dataset $p(\mathbf{x})$. (c) Inference result.

Consider modeling the complete data set $p(\mathbf{x}|z)$ under the assumption that the observations are independent and identically distributed (i.i.d.). Based on the Fig. 21.1(a), the joint distribution for a single observation $(\mathbf{x}_i, \mathbf{z}_i)$ given the model parameters $\boldsymbol{\theta}$ can be expressed:

$$p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) = \begin{cases} p(\mathcal{C}_1)p(\mathbf{x}_i|\mathcal{C}_1) & \text{if } z_i = 0 \\ p(\mathcal{C}_2)p(\mathbf{x}_i|\mathcal{C}_2) & \text{if } z_i = 1 \\ p(\mathcal{C}_3)p(\mathbf{x}_i|\mathcal{C}_3) & \text{if } z_i = 2 \end{cases}$$

Given N observations, the joint distribution for the entire dataset $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ along with their corresponding latent variables $\{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\}$ is:

$$p(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, \mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N|\boldsymbol{\theta}) = \prod_{n=1}^{N}\prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}$$

Here, $\pi_k = p(\mathcal{C}_k)$ represents the prior probability of the k-th component, and $p(\mathbf{x}_n|\mathcal{C}_k) =$

$\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ denotes the Gaussian distribution associated with component $\mathcal{C}_k$. Also, $z_{nk} \in \{0, 1\}$ and $\sum_k z_{nk} = 1$.

However, in practice, the latent variables $\mathbf{z}_k$ are often not directly observable, which complicates the modeling process.

In the following sections, we present various methods for identifying and handling these latent variables to improve the classification and modeling of data.

Chapter 22

Clustering

22.1 K-Means Clustering

Suppose that we have a data set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ consisting of N observations of a random D-dimensional variable $\mathbf{x} \in \mathbb{R}^D$. Our goal is to partition the data into K of clusters. Intuitively, a cluster can be thought as **a group of data points whose inter-point distances are small compared with the distances to points outside of the cluster**.

This notion can be formalized by introducing a set of D-dimensional vectors $\boldsymbol{\mu}_k$, which represents the centers of the clusters. Our goal is to find an assignment of data points to clusters, as well as a set of vectors $\{\boldsymbol{\mu}_k\}$. Objective function of K-means clustering (*distortion measure*) can be defined as follows:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} ||\boldsymbol{x}_n - \boldsymbol{\mu}_k||^2$$

, where $r_{nk} \in \{0, 1\}$ is a binary indicator variable which represents the **membership of data** $\mathbf{x}_n$. It can be expressed as follows:

$$r_{nk} = \begin{cases} 1 & \text{if } k = \text{argmin}_j \, ||\boldsymbol{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{otherwise} \end{cases}$$

Our goal is to find values for the $\boldsymbol{\mu}_k$ and the r_{nk} that minimize J.

We can minimize J through an iterative procedure in which each iteration involves two successive steps corresponding to successive optimizations with respect to the $\boldsymbol{\mu}_k$ and the r_{nk} First we choose some initial values for the $\boldsymbol{\mu}_k$. Then in the first phase we minimize J with respect to the r_{nk}, keeping the $\boldsymbol{\mu}_k$ fixed. In the second phase we minimize J with respect to the $\boldsymbol{\mu}_k$, keeping r_{nk} fixed. This two-stage optimization is then repeated until convergence.

Now consider the optimization of the $\boldsymbol{\mu}_k$ with the r_{nk} held fixed. The objective function J is a quadratic function of $\boldsymbol{\mu}_k$, and it can be minimized by setting its derivative with respect to $\boldsymbol{\mu}_k$ to zero giving

$$2 \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k) = 0.$$

We can arrange as

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\boldsymbol{x}_n}{\sum_n r_{nk}}.$$

The denominator of $\boldsymbol{\mu}_k$ is equal to the number of points assigned to cluster k. The mean of cluster k is essentially the same as the mean of data points $\mathbf{x}_n$ assigned to cluster k. For this reason, the procedure is known as the *K-means clustering algorithm.*

The two phases of re-assigning data points to clusters and re-computing the cluster means are repeated in turn until there is no further change in the assignments. These two phases reduce the value of the objective function J, so the convergence of the algorithm is assured. However, it may converge to a local rather than global minimum of J.

We can also sequentially update the μ_k as follows:

$$\mu_{k+1} = \mu_k + \eta(\mathbf{x}_k - \mu_k)$$

There are some properties to note:

- It is a hard clustering algorithm ($\leftrightarrow$ soft clustering)
- It is sensitive to the initialization of centroid.
- The number of clusters is uncertain.
- Sensitive to distance metrics (*e.g.,* Euclidean?)

22.2 Gaussian Mixture Models

K-means clustering is a form of hard clustering, where each data point is assigned to exactly one cluster. However, in some cases, soft clustering—where data points can belong to multiple clusters with varying degrees of membership—provides a better model in practice. A Gaussian Mixture Model (GMM) assumes a linear superposition of Gaussian components, offering a richer class of density models than a single Gaussian distribution.

In essence, rather than assuming that all data points are generated by a single Gaussian distribution, we assume that the data is generated by a mixture of K different Gaussian distributions, where each Gaussian represents a different component in the mixture.

For a single sample, the Gaussian Mixture Model can be expressed as a weighted sum of these individual Gaussian distributions:

$$\begin{aligned} p(\mathbf{x}) &= \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) \\ &= \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \end{aligned}$$

Here, $\mathbf{x}$ is a data point, π_k represents the mixing coefficients, $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ is a Gaussian distribution with mean $\boldsymbol{\mu}_k$ and covariance $\boldsymbol{\Sigma}_k$, and K is the number of Gaussian components.

A key quantity in GMMs is the conditional probability of $\mathbf{z}$ given $\mathbf{x}$, denoted as $p(z_k = 1|\mathbf{x})$ or $\gamma(z_k)$. This is also known as the responsibility or assignment probability, which represents the probability that a given data point $\mathbf{x}$ belongs to component k of the mixture. Essentially, this can be thought of as the **classification result** for $\mathbf{x}$.

This responsibility is updated using Bayes' Theorem, and can be expressed as:

$$\begin{aligned} \gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) &\equiv \frac{p(z_k = 1) p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1) p(\mathbf{x}|z_j = 1)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \end{aligned}$$

In this expression, π_k is the prior probability (or mixing coefficient) for component k, and $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ is the likelihood of the data point $\mathbf{x}$ under the Gaussian distribution corresponding to component k. The denominator is a normalization factor that ensures the responsibilities sum to 1 across all components for a given data point.

This framework allows for a soft classification of data points, where each point is associated with a probability of belonging to each cluster, rather than being strictly assigned to a single cluster as in K-means.

22.2.1 Maximum Likelihood

Suppose we have a data set of observations $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}^T \in \mathbb{R}^{N \times D}$ and we want to model the data distribution $p(\mathbf{X})$ using GMM. Assuming the data is independent and identically distributed

(i.i.d.), the likelihood of the entire dataset can be expressed as:

$$p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right).$$

To simplify the optimization process, we consider the log-likelihood function, which is given by:

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$

To solve the Maximum Likelihood Estimation (MLE) for Gaussian Mixture Models (GMMs), we typically consider the iterative *Expectation-Maximization* (EM) algorithm due to the non-convex nature of the problem. Before discussing how to maximize the likelihood, it is important to emphasize two significant issues that arise in GMMs: *singularities* and *identifiability*.

Singularity A major challenge in applying the maximum likelihood framework to Gaussian Mixture Models is the presence of singularities. This problem arises because the likelihood function can become unbounded under certain conditions, leading to an ill-posed optimization problem.

For simplicity, consider a Gaussian mixture model where each component has a covariance matrix of the form $\Sigma_k = \sigma_k^2 I$, where I is the identity matrix. Suppose one of the mixture components, say the j-th component, has its mean $\boldsymbol{\mu}_j$ exactly equal to one of the data points $\mathbf{x}_n$, so that $\boldsymbol{\mu}_j = \mathbf{x}_n$ for some value of n. The contribution of this data point to the likelihood function would then be:

$$\mathcal{N}(\mathbf{x}_n|\mathbf{x}_n, \sigma_j^2 I) = \frac{1}{\sqrt{2\pi}\sigma_j} \cdot \exp^0$$

As σ_j approaches 0, this term goes to infinity, causing the log-likelihood function to also diverge to infinity. Therefore, maximizing the log-likelihood function becomes an ill-posed problem because such singularities can always be present. These singularities occur whenever one of the Gaussian components **collapses** onto a specific data point, leading to a covariance matrix with a determinant approaching zero. This issue did not arise with a single Gaussian distribution because the variance cannot be zero by definition.

Identifiability Another issue in finding MLE solutions for GMMs is related to identifiability. For any given maximum likelihood solution, a GMM with K components has a total of $K!$ equivalent solutions. This arises from the fact that the $K!$ different ways of permuting the K sets of parameters (means, covariances, and mixing coefficients) yield the same likelihood.

In other words, for any point in the parameter space that represents a maximum likelihood solution, there are $K! - 1$ additional points that produce exactly the same probability distribution. This lack of identifiability means that the solution is not unique, complicating both the interpretation of the model and the optimization process.

22.2.2 Expectation Maximization for GMM

The goal of the Expectation-Maximization (EM) algorithm is to find maximum likelihood solutions for models that involve latent variables.

- Suppose that directly optimizing the likelihood $p(\mathbf{X}|\boldsymbol{\theta})$ is difficult.
- However, it is easier to optimize the complete-data likelihood function $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ as as discussed in the previous sections.
- In such cases, we can use the **EM algorithm**. EM algorithm is a general technique for finding maximum likelihood solutions in latent variable models.

Let's begin by writing down the conditions that must be satisfied at a maximum of the likelihood function. By setting the derivatives of $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ with respect to the means $\boldsymbol{\mu}_k$ of the Gaussian components to zero, we obtain

$$0 = -\sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

Multiplying by $\boldsymbol{\Sigma}_k^{-1}$ (which we assume to be non-singular) and rearranging we obtain

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n,$$

where we have defined

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}).$$

We can interpret N_k as the effective number of points assigned to cluster k. We can obtain the MLE solutions for other variables similarly.

Algorithm 2: EM algorithm for GMM

Initialize the means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k and evaluate the initial value of the log likelihood.

for n **do**

E-step: evaluate the responsibilities of $\mathbf{x}_n$ based on the current parameter values with the given parameters

$$\gamma(z_{nk}) = p(z_k = 1|\mathbf{x}_n) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

where z_{nk} denote the k-th component of $\mathbf{z}_n$

M-step: maximize expectation

- $\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$
- $\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^T$
- $\pi_k^{\text{new}} = p(z_k = 1) = \frac{N_k}{N}$

Evaluate the log likelihood to check for convergence of parameters

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$

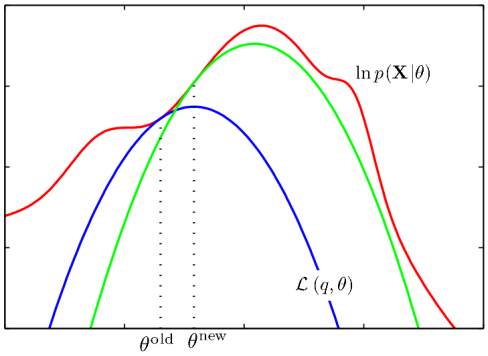


Figure 22.1: M-step of EM algorithm

22.3 Alternative View of EM

The goal of the EM algorithm is to find maximum likelihood (loglikelihood) solutions for models having latent variables.

$$\ln p(X|\theta) = ln \sum_Z p(X, Z|\theta).$$

We are not given the complete data set X, Z, but only the incomplete data X. Our state of knowledge of the values of the latent variables in Z is given only by the posterior distribution $p(Z|X, \theta)$. Because we cannot use the complete-data log likelihood function, we consider instead its expected value under the posterior distribution of the latent variable, which corresponds (as we shall see) to the E-step of the EM algorithm.

In the subsequent M-step, we maximize this expectation. If the current estimate for the parameters is denoted θ_{old}, then a pair of successive E- and M-steps gives rise to a revised estimate θ^{new}.

The algorithm is initialized by choosing some starting value for the parameters θ_0. The use of the expectation may seem somewhat arbitrary.

In the E-step, we use the current parameter values θ^{old} to find the posterior distribution of the latent variables given by $p(Z|X, \theta^{old})$. We then use this posterior distribution to find the **expectation of the complete-data log likelihood function** evaluated for some general parameter value θ. In other words, this is a expectation over a some function. This expectation, denoted $Q(\theta, \theta^{old})$, is given by

$$Q(\theta, \theta^{old}) = \sum_Z p(Z|X, \theta^{old}) \ln p(X, Z|\theta).$$

In the M-step, we determine the revised parameter estimate θ^{new} by maximizing this function

$$\theta^{new} = \operatorname{argmax} Q(\theta, \theta^{old}).$$

Algorithm 3: General EM algorithm

The goal is to maximize the likelihood function $p(X|\theta)$ with respect to θ given a joint distribution $p(X, Z|\theta)$.

1. Init θ^{old}
2. E-Step: evaluate $p(Z|X, \theta^{old})$
3. M-Step: evaluate θ^{new} given by

$$\theta^{new} = \operatorname{argmax} Q(\theta, \theta^{old}),$$

where

$$Q(\theta, \theta^{old}) = \sum_{Z} p(Z|X, \theta^{old}) \ln p(X, Z|\theta).$$

4. Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let

$$\theta^{old} \leftarrow \theta^{new}.$$

Return to the step 2.

22.4 Latent Variable Modeling

For each object x_i, we establish additional latent variable z_i which denotes the index of Gaussian from which i-th object was generated. Then our model is

$$p(X, Z|\theta) = \prod_{i=1}^{n} p(x_i, z_i|\theta) = \prod_{i=1}^{n} p(x_i|z_i, \theta)p(z_i|\theta) = \prod_{i=1}^{n} \mathcal{N}(x_i|\mu_{z_i}, \sigma_{z_i}^2)\pi_{z_i},$$

where $\pi_j = p(z_i = j)$ are prior probability of j-th gaussian and $\theta = \{\mu_j, \sigma_j, \pi_j\}_{j=1}^{K}$. If we know both X and Z then we can obtain explicit ML-solution:

$$\theta_{ML} = \underset{\theta}{\operatorname{argmax}}\, p(X, Z|\theta) = \underset{\theta}{\operatorname{argmax}} \log p(X, Z|\theta).$$

However, in practice, we don't know Z, but only know X. Thus, we need to maximize w.r.t. θ the log of incomplete likelihood

$$\begin{aligned}
\log p(X|\theta) &= \ln \int p(X, Z|\theta) dZ && (22.1)\\
&= \ln \int q(Z|X) \frac{p(X, Z|\theta)}{q(Z|X)} dZ && (22.2)\\
&\geq \underbrace{\int q(Z|X) \ln \frac{p(X, Z|\theta)}{q(Z|X)} dZ}_{\text{ELBO, } \mathcal{L}(q,\theta)} \quad \text{by Jensen's Inequality.} && (22.3)\\
&= \int q(Z|X) \ln p(X, Z|\theta) - q(Z|X) \ln q(Z|X) dZ && (22.4)\\
&= \int q(Z|X)[\ln p(X|Z, \theta) + \ln p(Z|\theta)] - q(Z|X) \ln q(Z|X) dZ && (22.5)\\
&= \int q(Z|X) \ln p(X|Z, \theta) - q(Z|X) \ln \frac{q(Z|X)}{p(Z|\theta)} dZ && (22.6)\\
&= \mathbb{E}_{q(Z|X)} \ln p(X|Z, \theta) - KL\left(q(Z|X) \| p(Z|\theta)\right) && (22.7)
\end{aligned}$$

To maximize the above equation, we need to minimize KL divergence.

To get more intuition about ELBO, we can express ELBO as follows:

$$\begin{aligned}
\mathcal{L}(\phi, \theta) &= \mathbb{E}_{q_\phi(z|x)} \left[\log \frac{p_\theta(x, z)}{q_\phi(z|x)} \right] \\
&= \mathbb{E}_{q_\phi(z|x)} \left[\log p_\theta(x, z) - \log q_\phi(z|x) \right] \\
&= \mathbb{E}_{q_\phi(z|x)} \left[\log p_\theta(x) + \log p_\theta(z|x) - \log q_\phi(z|x) \right] \\
&= \log p_\theta(x) - D_{\mathrm{KL}}(q_\phi(z|x) || p_\theta(z|x)) \\
&\leq \log p_\theta(x)
\end{aligned}$$

We can get a conclusion that maximizing ELBO is equivalent to minimizing the KL divergence through the above equation. Fianlly, the log-likelihood can be rewritten as follows:

$$\log p_\theta(x) = \mathcal{L}(\phi, \theta) + D_{\mathrm{KL}}(q_\phi(z|x) || p_\theta(z|x))$$

22.4.1 Expectation Maximization

We want to maximize ELBO, $\mathcal{L}(q, \theta)$ to minimize KL divergence between $q(Z)$ and $\log p(Z|X, \theta)$.

$$\max_{q,\theta} \mathcal{L}(q, \theta) = \max_{q,\theta} \int q(Z) \log \frac{p(X, Z|\theta)}{q(Z)} dZ.$$

We start from initial point θ_0 and iteratively repeat (*i*) E-step and (*ii*) M-step, iteratively:

- E-Step: θ_0 is fixed.

$$q(Z) = \operatorname*{argmax}_q \mathcal{L}(q, \theta) = \operatorname*{argmin}_q \mathrm{KL}(q(Z)|p(Z|X, \theta)) = p(Z|X, \theta_0).$$

  - This is because, maximizing ELBO is equal to minimizing KL divergence and the minimum q can be achieved when q is equal to $p(Z|X, \theta_0)$.
  - Now, we just have to evaluate $p(Z|X, \theta_0)$.

- M-Step: q is fixed.

$$\theta_* = \operatorname*{argmax}_\theta \mathcal{L}(q, \theta) = \operatorname*{argmax}_\theta \mathbb{E}_{q(Z)}[\log p(X, Z|\theta)]$$

  - Can be accomplished by taking derivatives
  - Set $\theta_0 = \theta_*$ and go to the E-Step until convergence

22.4.2 Categorical Latent Variables

$z_i \in \{1, ..., K\}$

$$p(x_i|\theta) = \sum_{k=1}^{K} p(x_i|k, \theta) p(z_i = k|\theta)$$

is simply a finite mixture of distributions.

E-Step:

$$q(z_i = k) = p(z_i = k|x_i, \theta) = \frac{p(x_k|z_i = k, \theta) p(z_i = k|\theta)}{\sum_{l=1}^{K} p(x_i|z_i = l, \theta) p(z_i = l|\theta)}$$

M-Step:

$$\operatorname*{argmax}_\theta \mathbb{E}_{q(Z)}[\log p(X, Z|\theta)] = \sum_{i=1}^{n} \mathbb{E}_{q(z_i)}[\log p(x_i, z_i|\theta)] = \sum_{i=1}^{n} \sum_{k=1}^{K} q(z_i = k) \log p(x_i, k|\theta)$$

For GMM, we model $p(x|z)$ as Gaussian.

Chapter 23

Hidden Markov Models

23.1 Introduction

The HMM is based on the Markov chain assumption. A Markov chain is a model that tells us something about the probabilities of sequences of random variables, states, each of which can take on values from some set. These sets can be words, or tags, or symbols representing anything, like the weather.

There are two important assumptions:

- Markov assumption
- Output independence: $p(x_i|z_1, \ldots, z_i, \ldots, z_T, x_1, \ldots, x_i, \ldots, x_T) = p(x_i|z_i)$

23.1.1 Conditional Independence

If two events A and B are **conditionally independent** given an event C then,

- $P(A \cap B|C) = P(A|C)P(B|C)$.
- $P(A|B, C) = P(A|C)$

23.1.2 Notation

- $X = (x_i, x_2, \ldots, x_T)$
- Initial state probabilities: $p(z_1) \sim \text{Multinomial}(\pi_1, ..., \pi_k)$, need to learn π
- Transition probability:

  $$p(z_t|z_{t-1} = i) \sim \text{Multinomial}(a_{i,1}, ..., a_{i,k})$$

  , where $a_{i,j} = p(z_t = j|z_{t-1} = i)$ and i and j denote clusters or states, respectively.
- Emission probability:

  $$p(x_t|z_t = i) \sim \text{Multinomial}(b_{i,1}, ..., b_{i,m})$$

  , where $b_{i,j} = p(x_t = j|z_t = i)$

23.2 Bayesian Network

23.2.1 Bayes Ball

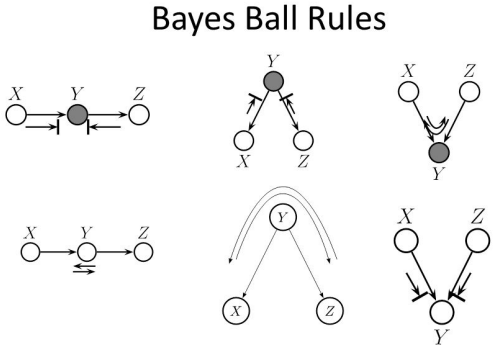


Figure 23.1: Bayes ball

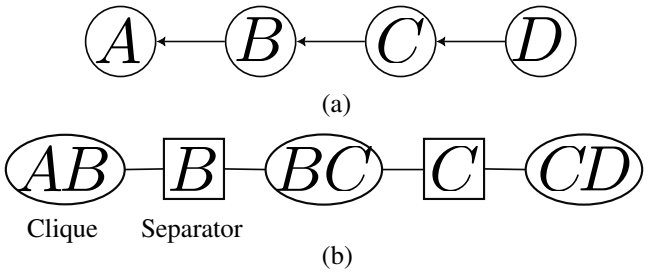
- Cascading: $P(Z|Y,X) = P(Z|Y)$. The information of Y decouples X and Z.
- Common parent: $P(X,Z|Y) = P(X|Y)P(Z|Y)$. The information of Y decouples X and Z.
- V-Structure (common child): Unlike the above two cases, the information of Y couples X and Z.

$$P(X,Y,Z) = P(X)P(Y)P(Y|X,Z).$$

23.2.2 Potential Function

Potential function is a function which is not a probability function, but it can become a probability function by normalizing it.

$$P(A,B,C,D) = P(A|B)P(B|C)P(C|D)P(D)$$



- Cliques: $\Psi(a,b), \Psi(b,c), \Psi(c,d)$
- Separators $\phi(b), \phi(c)$

Given a clique tree with cliques and separators, the joint probability distribution is defined as follows:

$$P(A,B,C,D) = P(U) = \frac{\prod_N \Psi(N)}{\prod_L \phi(L)} = \frac{\Psi(a,b)\Psi(b,c)\Psi(c,d)}{\phi(b)\phi(c)}$$

An effect of an observation propagates through the clique graph → **Belief propagation**. How to propagate the belief? **Absorption rule**!

Let's say we have some new observations about A, then it affects the clique $\Psi(a,b)$. The updated clique is now $\Psi^*(a,b)$. Similarly, $\phi^*(b) = \sum_A \Psi^*(a,b)$. Subsequently, $\Psi^*(b,c) = \Psi(b,c)\frac{\phi^*(b)}{\phi(b)}$.

23.3 Hidden Markov Models

Hidden Markov Models (HMMs) are a powerful statistical tool used for modeling sequences of observable events that are believed to be generated by underlying hidden states. The core idea behind HMMs is that the system being modeled can be represented as a **Markov process with unobservable (hidden) states z, where each state emits observable outputs x according to specific probability distributions**.

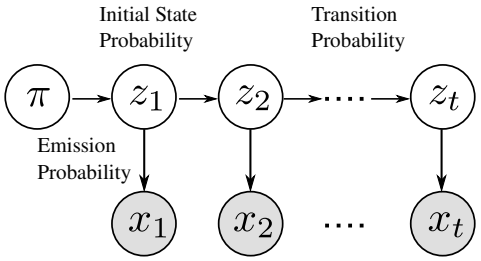


Figure 23.2: HMM Structure

In an HMM, the hidden states are connected by transition probabilities, which dictate the likelihood of moving from one state to another. Meanwhile, each state is associated with an emission probability, which defines the likelihood of observing a particular output given that state. The challenge and beauty of HMMs lie in their ability to infer the most probable sequence of hidden states that could have produced a given sequence of observations, even when the underlying states are not directly observable.

Through algorithms such as the Forward-Backward algorithm, the Viterbi algorithm, and the Baum-Welch algorithm, HMMs provide a framework for decoding sequences, estimating model parameters, and predicting future events based on past observations. In this post, we'll explore the fundamentals of Hidden Markov Models, their key components, and how they can be applied to solve real-world problems.

It's important to note that the observations in an HMM can be either discrete or continuous. When the latent factors are continuous, the model is often referred to as a *Kalman filter*.

23.3.1 Key Components of HMM

The key components of an HMM can be listed as follows:

- Initial state probability: $P(z_1) \sim \text{Mult}(\pi_1, \ldots, \pi_k)$. In other words, z is belong to one of k classes.
- Transition probability: $P(z_t|z^i_{t-1} = 1) \sim \text{Mult}(a_{i,1}, \ldots, a_{i,k})$,
  where $P(z^j_t = 1|z^i_{t-1} = 1) = a_{i,j}$
- Emission probability: $P(x_t|z^i_t = 1) \sim \text{Mult}(b_{i,1}, \ldots, b_{i,m}) \sim f(x_t|\theta_i)$,
  where $P(x^j_t = 1|z^i_t = 1) = b_{i,j}$. The probability of observing x_j at the i-th cluster.

Note that i and j are indices of clusters (*e.g.,* classes).

There are three main problems in HMM:

1. Evaluation Questions (likelihood):
   - Given $\boldsymbol{\pi}, \mathbf{a}, \mathbf{b}, X$
   - Find $p(X|M, \boldsymbol{\pi}, \mathbf{a}, \mathbf{b})$
   - How much are X likely to be observed by a model M?
2. Decoding Questions:
   - Given $\boldsymbol{\pi}, \mathbf{a}, \mathbf{b}, X$
   - Find $\text{argmax}_Z\, p(Z|X, M, \boldsymbol{\pi}, \mathbf{a}, \mathbf{b})$
   - What is the most probable sequence of Z (latent states)?
3. Learning Questions: Forward-Backward (Baum-Welch)
   - Given X
   - Find $\text{argmax}_{\boldsymbol{\pi},\mathbf{a},\mathbf{b}}\, p(X|M, \boldsymbol{\pi}, \mathbf{a}, \mathbf{b})$
   - What would be the optimal model parameters?

23.4 Evaluation: Forward-Backward Probability

23.4.1 Joint Probability

We can factorize the joint distribution of HMM in Fig. 23.2 by using a Bayesian approach as follows:.

$$p(X, Z) = p(x_1, \ldots, x_t, z_1, \ldots, z_t) \tag{23.1}$$
$$= p(z_1)p(x_1|z_1)p(z_2|z_1), \ldots, p(x_t|z_t)p(z_t|z_{t-1}) \tag{23.2}$$

The key assumption involved in factorizing the Markov chain within a Hidden Markov Model (HMM) is *conditional independence* among certain components of the state variables. Here's a detailed breakdown of what this assumption means:

- Independence of State Components: The transition of each component z_t^k only depends on its corresponding previous component z_{t-1}^k and is independent of other components.

As the number of latent factor increases, it is getting harder to decode the latent factors.

23.4.2 Marginal Probability

We want to compute the likelihood of sequence X which is given by

$$p(X|\boldsymbol{\pi}, \mathbf{a}, \mathbf{b}) = \sum_Z p(X, Z|\boldsymbol{\pi}, \mathbf{a}, \mathbf{b})$$

The computation can be done as follows:

$$\begin{aligned} p(X) &= \sum_Z p(X, Z) \\ &= \sum_{z_1} \cdots \sum_{z_t} p(x_1, \ldots, x_t, z_1, \ldots, z_t) \\ &= \sum_{z_1} \cdots \sum_{z_t} \pi_{z_1} \prod_{t=2}^{T} a_{z_{t-1}, z_t} \prod_{t=1}^{T} b_{z_t, x_t} \end{aligned}$$

The last step is done by using the factorization above. The computation of this equation requires lots of computations, so we will change it into a **recursive form** by using the factorization rule

$p(a, b, c) = p(a)p(b|a)p(c|a, b)$.

$$p(x_1, \ldots, x_t, z_t^k = 1) = \sum_{z_{t-1}} p(x_1, \ldots, x_{t-1}, x_t, z_{t-1}, z_t^k = 1) \tag{23.3}$$

$$= \sum_{z_{t-1}} p(\underbrace{x_1, \ldots, x_{t-1}, z_{t-1}}_{a}, \underbrace{x_t}_{c}, \underbrace{z_t^k = 1}_{b}) \tag{23.4}$$

$$= \sum_{z_{t-1}} p(x_1, \ldots, x_{t-1}, z_{t-1}) p(z_t^k = 1 | x_1, \ldots, x_{t-1}, z_{t-1}) p(x_t | z_t^k = 1, x_1, \ldots, x_{t-1}, z_{t-1}) \tag{23.5}$$

$\because p(a, b, c) = p(a)p(b|a)p(c|a, b)$ or by the structure of HMM

$$= \sum_{z_{t-1}} p(x_1, \ldots, x_{t-1}, z_{t-1}) p(z_t^k = 1 | z_{t-1}) p(x_t | z_t^k = 1) \tag{23.6}$$

$$= p(x_t | z_t^k = 1) \sum_{z_{t-1}} p(x_1, \ldots, x_{t-1}, z_{t-1}) p(z_t^k = 1 | z_{t-1}) \tag{23.7}$$

$$= b_{z_t^k, x_t} \sum_{z_{t-1}} p(x_1, \ldots, x_{t-1}, z_{t-1}) a_{z_{t-1}, z_t^k} \tag{23.8}$$

- In the second line, the x_{t-1} and z_{t-1} are grouped together.
- Then, we can find the HMM structure by factorizing the equation.
- In the fourth line, x terms are removed, since z_t only relies on z_{t-1} by the Markov assumption. Similarly, x_t only depends on z_t. We can interpret this by using Bayes ball too.

Now we can find a recursive structure of $p(x_1, \ldots, x_t, z_t^k = 1)$ as follows:

$$\alpha_t^k = p(x_1, \ldots, x_t, z_t^k = 1) = b_{k, x_t} \sum_i \alpha_{t-1}^i a_{i,k}$$

, where α_t^k **is the probabilities of being in state** k **after observing the first** t **observations.** Thus,

$$\begin{aligned} p(x_1, \ldots, x_t) &= \sum_{\mathbf{z}} p(x_1, \ldots, x_t, z) \\ &= \sum_k \alpha_t^k \end{aligned}$$

Note that α_t^k is also called **Forward probability**.

23.4.3 Forward Algorithm

Forward probability solves the evaluation problem. Essentially, this is a dynamic programming, so it calculates required values in a bottom-up manner.

- Forward probability: α_t^k, $Time \times States$

Note again that

$$p(X) = p(x_1, ..., x_T) = \sum_i \alpha_T^i = \sum_i p(x_1, ..., x_T, z_T^i = 1)$$

Note also that the forward-algorithm returns $p(X)$ and forward probability is the probability of being in state k after observing the first t observations without Z.

Algorithm 4: Forward Algorithm

Create a probability matrix $forward[M, T] = \alpha_t^k$
Initialization:
for *each state k=1,...,M* **do**
  $\alpha_1^k \leftarrow \pi_k b_{k,x_1}$
for *time step t=2,...,T* **do**
  for *each step k=1,...,M* **do**
    $\alpha_t^k = b_{k,x_t} \sum_i \alpha_{t-1}^i a_{i,k}$
Return $p(X) = \sum_i^M \alpha_T^i$

23.4.4 Backward Probability

The forward probability only considers an observation at t. To determine the z_t, we need to leverage the future observations. **The backward probability β is the probability of seeing the observations from time $t+i$ to the end, given that we are in state k at time t.**

$$\beta_t^k = p(x_{t+1}, \ldots, x_T | z_t^k = 1)$$

We want to compute $p(z_t^k = 1|X)$ rather than $p(x_1, \ldots, x_t, z_t^k = 1)$. In other words, we will leverage the whole observations X.

$$\begin{aligned} p(z_t^k = 1, X) &= p(x_1, \ldots, x_t, z_t^k = 1, x_{t+1}, \ldots, x_T) \\ &= p(x_1, \ldots, x_t, z_t^k = 1) p(x_{t+1}, \ldots, x_T | x_1, \ldots, x_t, z_t^k = 1) \\ &= p(x_1, \ldots, x_t, z_t^k = 1) p(x_{t+1}, \ldots, x_T | z_t^k = 1) \\ &= \alpha_t^k \beta_t^k \end{aligned}$$

We already know that $p(x_1, \ldots, x_t, z_t^k = 1) = \alpha_t^k$. We just need to compute backward probability as follows:

$$\begin{aligned} \beta_t^k &= p(x_{t+1}, \ldots, x_T | z_t^k = 1) \\ &= \sum_{z_{t+1}} p(\underbrace{z_{t+1}}_{a}, \underbrace{x_{t+1}}_{b}, \underbrace{x_{t+2}, \ldots, x_T}_{c} | z_t^k = 1) \\ &= \sum_i p(z_{t+1}^i = 1 | z_t^k = 1) p(x_{t+1} | z_{t+1}^i = 1, z_t^k = 1) p(x_{t+2}, \ldots, x_T | x_{t+1}, z_{t+1}^i = 1, z_t^k = 1) \\ &\because p(a, b, c) = p(a) p(b|a) p(c|a, b) \\ &= \sum_i p(z_{t+1}^i = 1 | z_t^k = 1) p(x_{t+1} | z_{t+1}^i = 1) p(x_{t+2}, \ldots, x_T | z_{t+1}^i = 1) \\ &= \sum_i a_{k,i} b_{i,x_{t+1}} \beta_{t+1}^i \end{aligned}$$

Another recursive structure:

$$\begin{aligned} p(z_t^k = 1, X) &= \alpha_t^k \beta_t^k \\ &= b_{k,x_t} \sum_i \alpha_{t-1}^i a_{i,k} \times \sum_i a_{k,i} b_{i,x_t} \beta_{t+1}^i \end{aligned}$$

This means at time t, the latent label is belong to some class k and this can be computed by using the forward probability and the backward probability. Now we can compute

$$p(z_t^k = 1|X) = \frac{p(z_t^k = 1, X)}{p(X)} = \frac{\alpha_t^k \beta_t^k}{p(X)}$$

Then,

$$k_t = \underset{k}{\operatorname{argmax}}\, p(z_t^k = 1|X)$$

Note that this is for a single latent variable at a single time step given the whole observation X, but we want to decode a sequence of latent variables. Thus, we need some decoding algorithm.

23.5 Decoding: Viterbi Algorithm

For any model, such as an HMM, that contains hidden variables, **the task of determining which sequence of variables is the underlying source of some sequence of observations is called the decoding task**.

We might propose to find the best sequence as follows:

1. For each possible hidden state sequence (HHH, HHC, HCH, etc.), we could run the forward algorithm and compute the likelihood of the observation sequence given that hidden state sequence.
2. Then, we could choose the hidden state sequence with the maximum observation likelihood.

However, this is not a feasible solution, because there are an exponentially large number of state sequences.

Instead, the most common decoding algorithms for HMMs is the **Viterbi algorithm**. Like the forward algorithm, **Viterbi** is a kind of **dynamic programming algorithm.**

Note that the Viterbi algorithm is identical to the forward algorithm except that it takes the **max** over the previous path probabilities whereas the forward algorithm takes the **sum**. This is because, we want to obtain **the most probable latent variable sequence**. Note also that the Viterbi algorithm has one component that the forward algorithm doesn't have: **backpointers**. The reason is that while the forward algorithm needs to produce an observation likelihood, the Viterbi algorithm must produce a probability and also the most likely state sequence. We compute this best state sequence by keeping track of the path of hidden states that led to each state and then at the end backtracing the best path to the beginning (the Viterbi backtrace).

We can leverage the forward-backward probabilities:

- $k^* = \text{argmax}_k \, p(z_t^k = 1|X) = \text{argmax}_k \, p(z_t^k = 1, X) = \text{argmax}_k \, \alpha_t^k \beta_t^k$

We will use a forward approach:

$$
\begin{aligned}
V_t^k &= \max_{z_1,\ldots,z_{t-1}} p(x_1, \ldots, x_{t-1}, z_1, \ldots, z_{t-1}, x_t, z_t^k = 1) && (23.9)\\
&= \max_{z_1,\ldots,z_{t-1}} p(x_t, z_t^k = 1|x_1, \ldots, x_{t-1}, z_1, \ldots, z_{t-1}) p(x_1, \ldots, x_{t-1}, z_1, \ldots, z_{t-1}) && (23.10)\\
&= \max_{z_1,\ldots,z_{t-1}} p(x_t, z_t^k = 1|z_{t-1}) p(x_1, \ldots, x_{t-2}, z_1, \ldots, z_{t-2}, x_{t-1}, z_{t-1}) && (23.11)\\
&= \max_{z_{t-1}} p(x_t, z_t^k = 1|z_{t-1}) \max_{z_1,\ldots,z_{t-2}} p(x_1, \ldots, x_{t-2}, z_1, \ldots, z_{t-2}, x_{t-1}, z_{t-1}) && (23.12)\\
&= \max_{i \in z_{t-1}} p(x_t, z_t^k = 1|z_{t-1}^i = 1) V_{t-1}^i && (23.13)\\
&= \max_{i \in z_{t-1}} p(x_t|z_t^k = 1) p(z_t^k = 1|z_{t-1}^i = 1) V_{t-1}^i && (23.14)\\
&= p(x_t|z_t^k = 1) \max_{i \in z_{t-1}} p(z_t^k = 1|z_{t-1}^i = 1) V_{t-1}^i && (23.15)\\
&= b_{k,x_t} \max_{i \in z_{t-1}} a_{i,k} V_{t-1}^i && (23.16)
\end{aligned}
$$

- V_t^k is Viterbi variable which denotes the probability that the HMM is in state k at t after observing the first t observations and $t-1$ latent variables. In another words, this is the probability of most likely sequence of states ending at state $z_t = k$.
- The first line assumes that the observation at time t and the latent variable are fixed and also the fourth line has the recursive structure.
- The third step, only z_{t-1} can affect the z_t, so we can remove all other unnecessary variables.
- The step six can be derived by the HMM structure.
- $i \in z_{t-1}$ simply denotes the index of potential cluster at $t-1$.
- We have already computed the backward and the forward probabilities. So we just need to apply the Viterbi algorithm.

Note that Also note that we present the most probable path by taking the maximum over all possible previous state sequences $\max_{z_1,\ldots,z_{t-1}}$. Like other DP-algorithm, Viterbi fills each cell recursively.

Algorithm 5: Viterbi Algorithm

$V_t^k = viterbi[M, T]$, where M is the number states
for *k=1,...,M* **do**
  $V_1^k \leftarrow \pi_{z_k} b_{k,x_1}$
  $backpointer[k, 1] \leftarrow 0$
for *t=2,...,T* **do**
  for *k=1,...,M* **do**
    $V_t^k \leftarrow b_{k,x_t} \max_{k'} V_t^{k'} a_{k',k}$, where k' is the previous state.
    $backpointer[k, t] \leftarrow b_{k,x_t} \operatorname{argmax}_{k'} V_t^{k'} a_{k',k}$
$bestpathprob \leftarrow \max_k V_T^k$ //termination step
$bestpathpointer \leftarrow \operatorname{argmax}_k V_T^k$ //termination step
$bestpath \leftarrow$ the path starting at state *bestpathpointer*, that follows backpointer[] to states back in time
Return *bestpathpointer*, *bestpathprob*

Viterbi algorithm typically shows some technical issues:

- Underflow problems $\rightarrow \log V$.

23.6 Learning: Baum-Welch Algorithm

We have to learn HMM parameters with only X. Baum-Welch algorithm or Forward-Backward Algorithm is a standard training algorithm for HMM. The algorithm let us train both the transition and the emission probabilities of the HMM. If we do not have the information about Z, then we can assign the most probable Z given X.

- Given X, estimate parameters π, a, b.
- Then, find the most probable Z given the parameters.

We will use EM algorithm!

23.6.1 EM Algorithm

$$P(X|\theta) = \sum_Z P(X, Z|\theta) \rightarrow \ln P(X|\theta) = \ln \sum_Z P(X, Z|\theta).$$

We cannot directly estimate the log-likelihood function, so we will estimate the expectation of it.

$$\begin{aligned} Q(\theta, \theta^{old}) &= \mathbb{E}_Z \ln P(X, Z|\theta) \\ &= \sum_Z p(Z|X, \theta^{old}) \ln P(X, Z|\theta) \\ &= \sum_Z p(Z|X, \pi^t, a^t, b^t) \ln P(X, Z|\pi, a, b). \end{aligned}$$

Note that $p(X, Z) = \pi_{z_1} \prod_{t=2}^T a_{z_{t-1}, z_t} \prod_{t=2}^T b_{z_t, x_t}$. Thus, $\ln p(X, Z) = \ln \pi_{z_1} + \sum_{t=2}^T \ln a_{z_{t-1}, z_t} + \sum_{t=1}^T \ln b_{z_t, x_t}$. Therefore

$$Q(\theta, \theta^{old}) = \sum_Z p(Z|X, \theta^{old}) \bigg(\ln \pi_{z_1} + \sum_{t=2}^T \ln a_{z_{t-1}, z_t} + \sum_{t=1}^T \ln b_{z_t, x_t} \bigg).$$

To optimize the above function we will use the Lagrange method as follows:

$$\mathcal{L}(\pi, a, b) = Q(\theta, \theta^{old}) - \lambda_\pi \bigg(\sum_{i=1}^K \pi_i - 1 \bigg) - \sum_i^K \lambda_{a_i} \bigg(\sum_{j=1}^K a_{i,j} - 1 \bigg) - \sum_i^K \lambda_{b_i} \bigg(\sum_{j=1}^K b_{i,j} - 1 \bigg).$$

The constraints are for forcing the sum of each probability is equal to 1.

Now, take a partial derivative for each parameter. Let's take a derivative with regard to π_i first. Then,

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \pi_i} &= \frac{\partial Q(\theta, \theta^{old})}{\partial \pi_i} - \lambda_\pi \\ &= \frac{\partial}{\partial \pi_i} \sum_Z p(Z|X, \theta^{old}) \ln \pi_{z_1} - \lambda_\pi \\ &= \frac{p(z_1^i = 1|X, \theta^{old})}{\pi_i} - \lambda_\pi \\ \frac{\partial \mathcal{L}}{\partial \lambda_{\pi_i}} &= \sum_{i=1}^K \pi_i - 1 = 0 \rightarrow \sum_{i=1}^K \pi_i = 1. \end{aligned}$$

By setting the derivative is equal to zero,

$$\pi_i = \frac{p(z_1^i = 1|X, \theta^{old})}{\lambda_\pi}.$$

By using the constraint of π, the Lagrange multiplier λ_π must be a normalizer.

$$\pi_i = \frac{p(z_1^i = 1|X, \theta^{old})}{\sum_{j=1}^{K} p(z_1^j = 1|X, \theta^{old})}.$$

Similarly, we can compute other parameters too.

$$a_{i,j}^{t+1} = \frac{\sum_{t=2}^{T} p(z_{t-1}^i = 1, z_t^j = 1|X, \theta^{old})}{\sum_{t=2}^{T} p(z_{t-1}^i = 1|X, \theta^{old})}.$$
$$b_{i,j}^{t+1} = \frac{\sum_{t=1}^{T} p(z_{t1}^i = 1|X, \theta^{old}) I(x_t = j)}{\sum_{t=1}^{T} p(z_t^i = 1|X, \theta^{old})},$$

where $I(x)$ is an indicator function which returns 1 if x is true and 0, otherwise.

23.7 Python Implementation

23.7.1 Viterbi Algorithm

The Viterbi algorithm is a dynamic programming algorithm used to determine the most probable sequence of hidden states in a Hidden Markov Model (HMM) based on a sequence of observations.

The algorithm works by recursively computing the probability of the most likely sequence of hidden states that ends in each state for each observation.

At each time step, the algorithm computes the probability of being in each state and emits the current observation based on the probabilities of being in the previous states and making a transition to the current state.

Assuming we have an HMM with N hidden states and T observations, the Viterbi algorithm can be summarized as follows:

Initialization: At time t=1, we set the probability of the most likely path ending in state i for each state i to the product of the initial state probability pi and the emission probability of the first observation given state i. This is denoted by: delta[1,i] = pi * b[i,1]. Recursion: For each time step t from 2 to T, and for each state i, we compute the probability of the most likely path ending in state i at time t by considering all possible paths that could have led to state i. This probability is given by:

$$delta[t, i] = max_j(delta[t-1, j] * a[j, i] * b[i, t])$$

Here, a[j,i] is the probability of transitioning from state j to state i, and b[i,t] is the probability of observing the t-th observation given state I.

We also keep track of the most likely previous state that led to the current state i, which is given by:

$$psi[t, i] = argmax_j(delta[t-1, j] * a[j, i])$$

- Termination: The probability of the most likely path overall is given by the maximum of the probabilities of the most likely paths ending in each state at time T. That is, $P* = max_i(delta[T, i])$.
- Backtracking: Starting from the state $i*$ that gave the maximum probability at time T, we recursively follow the psi values back to time $t = 1$ to obtain the most likely path of hidden states.

The Viterbi algorithm is an efficient and powerful tool that can handle long sequences of observations using dynamic programming.

23.8 Summary

- Forward-probability: probability of being in state k after observing the first t observations.

$$\alpha_t^k = p(x_1, ..., x_t, z_t^k = 1)$$

- Backward-probability: probability of observations from time $t+1$ to the end, given that we are in state k

$$\beta_t^k = p(x_{t+1}, ..., x_T | z_t^k = 1)$$

- These two sets of probability distributions can then be combined to obtain the distribution over states at any specific point in time given the entire observation sequence

$$\begin{aligned} p(z_t^k = 1, X) &= p(x_1, ..., x_t, z_t^k = 1, x_{t+1}, ..., x_T) \\ &= p(x_1, ..., x_t, z_t^k = 1) p(x_{t+1}, ..., x_T | x_1, ..., x_t, z_t^k = 1) \\ &= p(x_1, ..., x_t, z_t^k = 1) p(x_{t+1}, ..., x_T | z_t^k = 1) \\ &= \alpha_t^k \beta_t^k \end{aligned}$$

  In short, if we know the forward and backward probability, we could know the cluster of state at time t given our observations.

- Forward-algorithm: return a marginal likelihood of the observed sequence
- Forward-backward: predict a single hidden state
- Viterbi: predict an entire sequence of hidden states
- Baum-Welch: unsupervised training (EM)

There are two shortcomings of HMM:

- HMM models capture dependences between each state and only its corresponding observation: Most NLP cases, many tasks needs not only local but also global feature (sentence level).
- Mismatch between learning objective function and prediction objective function: HMM learns a joint distribution of states and observations $p(Y, X)$, but we are more interested in $p(Y|X)$

Chapter 24

Explicit Generative Models

24.1 Variational Autoencoder

Our goal is to find the data distribution $p(X)$. Fig. 24.1 represents a general structure of deep generative model. As you can see, we first sample $z \sim p(z)$ and feed it into a deep neural network $f(z)$ and output x.

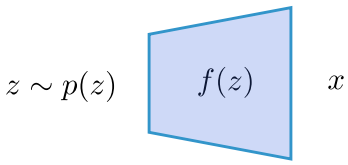


Figure 24.1: General structure of deep generative models. This model does not infer z from x.

VAE performs an inference by introducing a probabilistic encoder, called inference network. VAEs are generative model with a latent variable distributed according to some distribution $p(z_i)$. The observed variable is distributed according to a conditional distribution

$$p_\theta(x_i|z_i)$$

This conditioning means the latent variable values are the one most likely given the observations. We also create a distribution $q_\phi(z_i|x_i)$. We would like to be able to encode our data into the latent variable space. Let's model the distribution.

- $p_\theta(x_i|z_i) \sim \mathcal{N}(x_i|\mu(z_i), \sigma^2(z_i))$: A probabilistic decoder (or generative network, θ)
- $q_\phi(z_i|x_i)$: A probabilistic encoder (or inference network ϕ). We can choose a family of distributions for our conditional distribution q (*e.g.,* standard Gaussian distribution).

  $$q_\phi(z_i|x_i) = \mathcal{N}(z_i|\mu(x_i, W_1), \sigma^2(x_i, W_2)I),$$

  where W_1 and W_2 are network weights and collectively denoted as ϕ. We create a neural network to model the distribution q from our data in a non-linear manner. The outputs of the network are μ and σ.

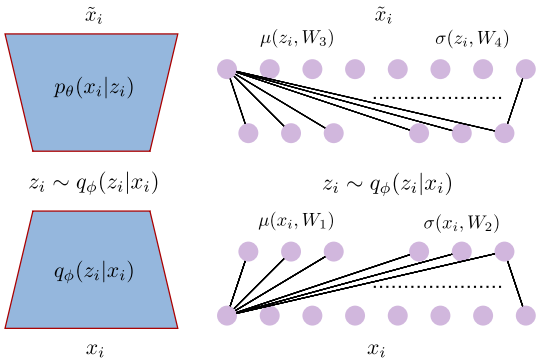


Figure 24.2: Overview of variational autoencoder.

$$
\begin{aligned}
p(X, Z|\theta) &= \prod_{i=1}^{n} \underbrace{p(x_i|z_i, \theta)}_{\text{Likelihood, Generator}} \underbrace{p(z_i|\theta)}_{\text{Prior on latent variable}} \\
&= \prod_{i=1}^{n} \mathcal{N}(x_i| \underbrace{\mu(z_i), \sigma^2(z_i))}_{\text{Non-linear}} \mathcal{N}(z_i|0, I)
\end{aligned}
$$

Subsequently, marginal distributions can be expressed as follows under i.i.d. assumption:

$$
\begin{aligned}
p(X|\theta) &= \prod_{i=1}^{n} p(x_i|\theta) \\
&= \prod_{i=1}^{n} \int p(x_i, z_j|\theta) dz_j \\
&= \prod_{i=1}^{n} \int p(x_i|z_i, \theta) p(z_i|\theta) dz_i \\
&= \prod_{i=1}^{n} \int \mathcal{N}(x_i|\mu(z_i), \sigma^2(z_i)) \underbrace{\mathcal{N}(z_i|0, I)}_{\text{Mixture weight}} dz_i
\end{aligned}
$$

- As you can see, the marginal distribution $p(X|\theta)$ becomes a mixture of Gaussian (infinite mixture of Gaussian).
- Even though $p(x|z)$ and $p(z)$ are normal, $p(x)$ is not normal, because it is a mixture distribution.
- The non-linearity of Gaussian parameters (modeled by a neural network), conjugacy between the prior and the likelihood does not hold anymore.
- Again, μ and σ is non-linear function of z modeled by some non-linear neural network. The neural network works as a powerful non-linear parameter approximator (based on universal approximation theorem).
- Simple prior is used. Let's consider the data x is an image of 100×100 pixels. Then the covariance matrix has to be 10000×10000. Thus, it is common to set a simple prior such as the standard Gaussian (covariance matrix is diagonal matrix). However, even if we set a simple distribution, with the infinite mixture of Gaussian, we can model any distribution.

- VAE uses a global parametric model to predict the local variational parameters for each data point (**amortized inference**).
- It allows to convert complicated large-dimensional data distributions into simple lower-dimensional latent variable representations.

24.1.1 VAE Optimization

We can train VAE using variational inference with the following objective function, ELBO:

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - D_{\mathrm{KL}}(q_\phi(z|x)||p_\theta(z))$$

Let's closely look at this objective function:

- In $q_\phi(z|x)$, x is a given data, so it is not stochatic. How to sample z?
- q has to be deterministic and differentiable.

  $\rightarrow$ **Reparameterization trick**!

  $$\tilde{z} \sim q_\phi(z|x) \rightarrow \tilde{z} \sim g_\phi(\epsilon, x)$$

  , where $\epsilon \sim p(\epsilon)$.
- Estimated by using Monte-Carlo estimation

  $$\mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] \approx \frac{1}{N} \sum_j \log p_\theta(x_i|z_j).$$

24.1.2 Conditional VAE

If we have label information about data, then it would provide a better optimization of VAE model. Recall that the following objective function is the objective of the original VAE:

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - D_{\mathrm{KL}}(q_\phi(z|x)||p_\theta(z))$$

In conditional VAE,

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q_\phi(z|x,y)}[\log p_\theta(x|y, z)] - D_{\mathrm{KL}}(q_\phi(z|x, y) \;||\; p_\theta(z|y))$$

$$\log p(X|Y) = \ln \int q(Z|X, Y) \frac{p(X, Z|Y)}{q(Z|X, Y)} dZ \tag{24.1}$$

$$\geq \underbrace{\int q(Z|X, Y) \ln \frac{p(X, Z|Y)}{q(Z|X, Y)} dZ}_{\text{ELBO, } \mathcal{L}(q,\theta)} \quad \text{by Jensen's Inequality.} \tag{24.2}$$

$$\ldots \tag{24.3}$$

$$\ldots \tag{24.4}$$

$$= \mathbb{E}_{q(Z|X,Y)}[\ln p(X|Z, Y)] - KL(q(Z|X, Y)||p(Z|Y)) \tag{24.5}$$

Note that not we have a prior $p_\theta(z|y)$. However, we have no idea about latent variable z, so we simply assume that we cannot impact the z by y. Thus, we typically set it as a standard normal distribution. Also, we can simply concatenate the input X with Y.

24.1.3 Variational Deep Embedding (VaDE)

The generative process of VADE $p(x, z, c) = p(x|z)p(z|c)p(c)$:

- Choose a cluster $c \sim Cat(\pi)$
- Choose a latent vector $z \sim \mathcal{N}(\mu_c, \sigma_c^2 I)$
- Choose a sample x:

$$x \sim \begin{cases} Ber(\mu_x) & \text{If x is binary} \\ \mathcal{N}(\mu_x, \sigma_x^2 I) & \text{else} \end{cases}$$

ELBO of VaDE:

$$\log p(X) = \ln \int \sum_c p(X, Z, C) dz \tag{24.6}$$

$$\geq \underbrace{\int q(Z, C|X) \ln \frac{p(X, Z, C)}{q(Z, C|X)} dZ}_{\text{ELBO}} \tag{24.7}$$

The ELBO can be decomposed as follows:

$$\begin{aligned} \mathcal{L}_{ELBO} &= \mathbb{E}_q(z, c|x) \left[\ln \frac{p(x, z, c)}{q(z, c|x)} \right] \\ &= \mathbb{E}_q(z, c|x)[\ln p(x, z, c) - \ln q(z, c|x)] \\ &= \mathbb{E}_q(z, c|x)[\ln p(x|z) + \ln p(z|c) + \ln p(c) - \ln q(z|x) - \ln q(c|x)] \end{aligned}$$

By using two factorizations:

- $p(x, z, c) = p(x|z)p(z|c)p(c)$
- $q(z, c|x) \approx q(z|x)q(c|x)$ (Mean-field assumption)
  - $q(z|x) \sim \mathcal{N}$: encoder, estimate mean and variance.
  - $q(c|x)$: assignment probability of Gaussian mixture model

24.1.4 Importance Weighted VAE

Chapter 25

Implicit Generative Models

25.1 Generative Adversarial Networks

- Generator's distribution: p_g
- Prior on input noise: $p_z(z)$
- Mapping to data space: $z \to x$ through $G(z; \theta_g)$

  a differentiable multilayer perceptron with parameter θ_g
- $D(x; \theta_d)$: a differentiable multilayer perceptron with parameter θ_d. It outputs a single scalar
- $D(x)$: probability that x (real) came from the data rather than p_g (fake)

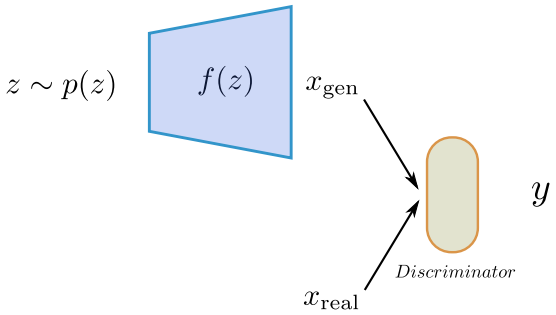


Figure 25.1: GAN structure

25.1.1 Discriminator

The discriminator's goal is to maximize the following equation given G

$$\mathbb{E}_{x \sim p_{data}(x)} \log(D(x)) + \mathbb{E}_{z \sim p_z(z)} \log(1 - D(G(z)))$$

The optimal discriminator given G can be denoted as D^*_G. To get the optimal discriminator, define a value function

$$V(G, D) := \mathbb{E}_{x \sim p_{data}(x)} \log(D(x)) + \mathbb{E}_{z \sim p_z(z)} \log(1 - D(G(z))).$$

Then, $D_G^* = \text{argmax}_D V(G, D)$

However, the generator G wants to minimize the value function given $D = D_G^*$.

$$G^* = \text{argmin}_G V(G, D_G^*).$$

$$\min_G \max_D V(D, G) = \mathbb{E}_{x \sim p_{data}(x)}[\log D(x)] + \mathbb{E}_{z \sim p_z(z)}[\log(1 - D(G(z)))]$$

- $\min_G \rightarrow$ try to generate fake data that is similar to real data
- $\max_D \rightarrow$ try to assign correct label [1]

At this point, we must show that this optimization problem has a unique solution G^* and that this solution satisfies $p_G = p_{data}$.

One big idea from the GAN paper–, which is different from other approaches is that G **need not be invertible**. Many pieces of notes online miss this fact when they try to replicate the proof and incorrectly use the change of variables formula from calculus (which would depend on G being invertible). Rather, the whole proof relies on this equality:

$$\mathbb{E}_{z \sim p_z(z)} \log(1 - D(G(z))) = \mathbb{E}_{x \sim p_G(x)} \log(1 - D(x)).$$

With the above equality,

$$\begin{aligned}
&\mathbb{E}_{x \sim p_{data}(x)} \log(D(x)) + \mathbb{E}_{z \sim p_z(z)} \log(1 - D(G(z))) \\
&= \int_x p_{data}(x) \log D(x) \, \mathrm{d}x + \int_z p(z) \log(1 - D(G(z))) \, \mathrm{d}z \\
&= \int_x p_{data}(x) \log D(x) + p_G(x) \log(1 - D(x)) \, \mathrm{d}x
\end{aligned}$$

Additionally, we will use the following property:

$$f(y) = a \log y + b \log(1 - y).$$

To find a critical point,

$$f'(y) = 0 \Rightarrow \frac{a}{y} - \frac{b}{1 - y} = 0 \Rightarrow y = \frac{a}{a + b}$$

If $a + b \neq 0$, do the second derivative test:

$$f''\big(\frac{a}{a+b}\big) = -\frac{a}{(\frac{a}{a+b})^2} - \frac{b}{(1 - \frac{a}{a+b})^2} < 0$$

If $a, b \in (0, 1)$, $\frac{a}{a+b}$ is a maximum.

By rewriting the equation,

$$\begin{aligned}
V(G, D) &= \int_x p_{data}(x) \log D(x) + p_G(x) \log(1 - D(x)) \, \mathrm{d}x \\
&\leq \int_x \max_y p_{data}(x) \log y + p_G(x) \log(1 - y) \, \mathrm{d}x
\end{aligned}$$

Thus, if $D(x) = \frac{p_{data}}{p_{data} + p_G}$, then we can achieve the maximum $V(G, D)$.

[1] The above equation is trained separately at the same time, don't get confused

25.1.2 Generator

If we achieve the optimal G (i.e., $p_G = p_{data}$), then D would be completely confused and $D^*_G(x) = \frac{p_{data}}{p_{data}+p_G} = \frac{1}{2}$ (it means that D cannot make a clear decision.).

The global minimum of the virtual training criterion $C(G) = \max_D V(G, D)$ is acheived if and only if $p_G = p_{data}$. Let's plug $D^*_G(x)$ into the criterion then,

$$C(G) = \int_x p_{data}(x) \log \big(\frac{p_{data}(x)}{p_G(x) + p_{data}(x)}\big) + p_G(x) \log \big(\frac{p_G(x)}{p_G(x) + p_{data}(x)}\big)\, \mathrm{d}x.$$

To get the minimum $C(G)$, we can use the Jansen-Shannon divergence:

$$\begin{aligned}
D_{JS}(p_{data}||p_G) &= \frac{1}{2}\left[D_{KL}\Big(p_{data}\Big|\Big|\frac{p_{data}+p_G}{2}\Big) + D_{KL}\Big(p_G\Big|\Big|\frac{p_{data}+p_G}{2}\Big)\right] \\
&= \frac{1}{2}\left[\left(\int_x p_{data}(x)\log\left(\frac{2p_{data}(x)}{p_{data}(x)+p_G(x)}\right)dx\right) + \left(\int_x p_G(x)\log\left(\frac{2p_G(x)}{p_{data}(x)+p_G(x)}\right)dx\right)\right] \\
&= \frac{1}{2}\left[\left(\int_x p_{data}(x)\log 2 + p_{data}(x)\log\left(\frac{p_{data}(x)}{p_{data}(x)+p_G(x)}\right)dx\right) + \right. \\
&\qquad \left.\left(\int_x p_G(x)\log 2 + p_G(x)\log\left(\frac{p_G(x)}{p_{data}(x)+p_G(x)}\right)dx\right)\right] \\
&= \frac{1}{2}\left[\left(\log 2 + \int_x p_{data}(x)\log\left(\frac{2p_{data}(x)}{p_{data}(x)+p_G(x)}\right)dx\right) + \right. \\
&\qquad \left.\left(\log 2 + \int_x p_G(x)\log\left(\frac{2p_G(x)}{p_{data}(x)+p_G(x)}\right)dx\right)\right] \\
&= \frac{1}{2}(\log 4 + C(G))
\end{aligned}$$

Thus,

$$C(G) = -\log 4 + 2D_{JS}(p_{data}||p_G)$$

Since the Jensen-Shannon divergence between two distributions is always non-negative and zero only when they are equal, we have shown that $C^* = -\log(4)$ is the global minimum of $C(G)$ and that the only solution is $p_G = p_{data}$, i.e., the generative model perfectly replicating the data generating process.

25.2 Some notes

What would be the optimal discriminator that separates the two different distributions $p(x)$ and $q(x)$? It turns out that it is

$$f(x) = \frac{q(x)}{p(x) + q(x)}$$

Actually, there are many choices for classifiers e.g., KL-divergence

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**
  for k steps **do**
    • Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
    • Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
    • Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)\right].$$

  end for
  • Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  • Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for
The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

Figure 25.2: Training GAN

1. What do we need to learn a classifier?

   - Only samples from $p(x)$ and $q(x)$

2. How do we parameterize $q(x)$?

   - Parametric density function (Gaussian)
   - Define implicitly (GANs approach): define mapping from one (noise) to another (data or image)

The orignal GAN does not learn the data distributions.

25.3 Wasserstein Generative Adversarial Networks

25.3.1 KL Divergence

Definition:

$$D_{\mathrm{KL}}(q(x)||p(x)) = \int q(x) \log \frac{q(x)}{p(x)} dx$$

- Forward KL:
  - If $q(z) \to 0, \text{Forward KL} \to \infty$
  - Zero avoiding for $q(z)$
- Reverse KL:
  - If $p(z) \to 0, \text{Reverse KL} \to \infty$
  - Zero forcing: $q(z) \to 0$

Typically, $p(x)$ and $q(x)$ are far apart at the initial state.

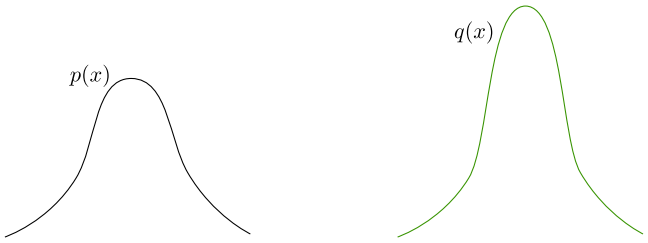


Figure 25.3: Two distributions: $p(x)$ and $q(x)$

Thus, both the forward KL and the reverse KL suffers an unstability issue. Specifically, in each case, if the denominator goes to zero, then the divergence goes to infinity.

25.3.2 Jensen-Shannon Divergence

Definition:

$$D_{JS}(p_{data}||p_G) = \frac{1}{2}\left[D_{KL}\left(p_{data}\middle|\middle|\frac{p_{data}+p_G}{2}\right) + D_{KL}\left(p_G\middle|\middle|\frac{p_{data}+p_G}{2}\right)\right]$$

The KL divergence's issue can be alleviated by JS-divergence. Consider a simple example in Fig. 25.46

$$\forall (x,y) \in P, x = 0 \text{ and } y \sim U(0,1)$$
$$\forall (x,y) \in Q, x = \theta, 0 \leq \theta \leq 1 \text{ and } y \sim U(0,1)$$

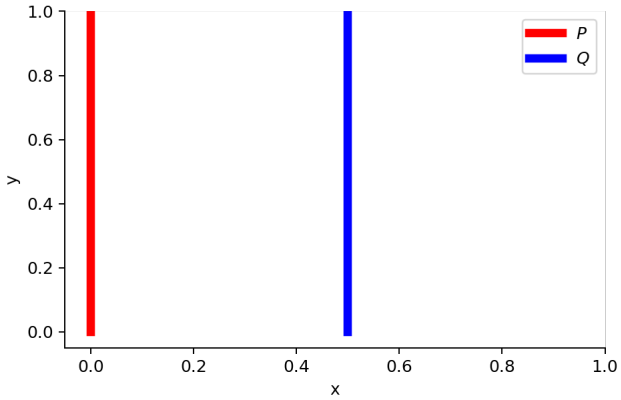


Figure 25.4: Two distributions: $p(x)$ and $q(x)$

$$
\begin{aligned}
D_{\mathrm{KL}}(q(x)||p(x)) &= \infty \\
D_{\mathrm{KL}}(p(x)||q(x)) &= \infty \\
D_{JS}(p_{data}||p_G) &= \frac{1}{2}\left[D_{KL}\left(p_{data}\middle|\middle|\frac{p_{data}+p_G}{2}\right) + D_{KL}\left(p_G\middle|\middle|\frac{p_{data}+p_G}{2}\right)\right] \\
&= \frac{1}{2}\left[D_{KL}\left(p_{data}\middle|\middle|\frac{p_{data}}{2}\right) + +D_{KL}\left(p_G\middle|\middle|\frac{p_G}{2}\right)\right] \\
&= \frac{1}{2}[\log 2 + \log 2] = \log 2 \\
W(p,q) &= |\theta|
\end{aligned}
$$

Therefore, Jensen-Shannon divergence is more stabler than KL divergece. This is one of the reasons why GAN, which uses JS divergence works better than VAE, which uses KL divergence.

However, JS divergence also has some problem. If the value is close to $\frac{1}{2}\log 2$, then the gradient will be very small or close to zero, because the divergence is close to constant. It means that a training speed is very slow. Thus, we need a better metric.

25.3.3 Wasserstein Distance

Wasserstein Distance is a measure of the distance between two probability distributions. It is also called Earth Mover's distance, short for EM distance, because informally it can be interpreted as the minimum energy cost of moving and transforming a pile of dirt in the shape of one probability distribution to the shape of the other distribution.

$$W(p_r, p_g) = \inf_{\gamma \sim \Pi(p_r, p_g)} \mathbb{E}_{(x,y)\sim\gamma}[\|x-y\|]$$

- Π: is the transportation plan and the set of all possible joint probability distributions between p_r and p_g. One joint distribution $\gamma \sim \Pi(p_r, p_g)$ describes one transport plan.
- $\mathbb{E}_{x,y\sim\gamma}\|x-y\| = \sum_{x,y}\gamma(x,y)\|x-y\|$

- Finally, we take the minimum one among the costs of all dirt moving solutions as the EM distance (by infimum).

25.4 WGAN

However, consider all possible joint distribution is intractable, so dual solution can be used.

$$W(p_r, p_g) = \frac{1}{K} \sup_{\|f\|_L \leq K} \mathbb{E}_{x \sim p_r}[f(x)] - \mathbb{E}_{x \sim p_g}[f(x)]$$

So to calculate the Wasserstein distance, we just need to find a 1-Lipschitz function. To enforce the constraint, WGAN applies a very simple clipping to restrict the maximum weight value in f, i.e. the weights of the discriminator

Suppose this function f comes from a family of K-Lipschitz continuous functions, $\{f_w\}_{w \in W}$, parameterized by w. In the modified Wasserstein-GAN, the "discriminator" model is used to learn w to find a good f_w and the loss function is configured as measuring the Wasserstein distance between p_r and p_g.

$$L(p_r, p_g) = W(p_r, p_g) = \max_{w \in W} \mathbb{E}_{x \sim p_r}[f_w(x)] - \mathbb{E}_{z \sim p_r(z)}[f_w(g_\theta(z))]$$

There are two ways to satisfy the Lipschitz continuity:

- Weight clipping
- Gradient Penalty

25.4.1 Lipschitz continuity

The function f in the new form of Wasserstein metric is demanded to satisfy $\|f\|_L \leq K$, meaning it should be K-Lipschitz continuous.

A real-valued function $f : \mathbb{R} \to \mathbb{R}$ is called K-Lipschitz continuous if there exists a real constant $K \geq 0$ such that, for all $x_1, x_2 \in \mathbb{R}$

$$|f(x_1) - f(x_2)| \leq K|x_1 - x_2|$$

Here K is known as a Lipschitz constant for function $f(\cdot)$. Functions that are everywhere continuously differentiable is Lipschitz continuous, because the derivative, estimated as $\frac{|f(x_1)-f(x_2)|}{|x_1-x_2|}$, has bounds. However, a Lipschitz continuous function may not be everywhere differentiable, such as $f(x) = |x|$

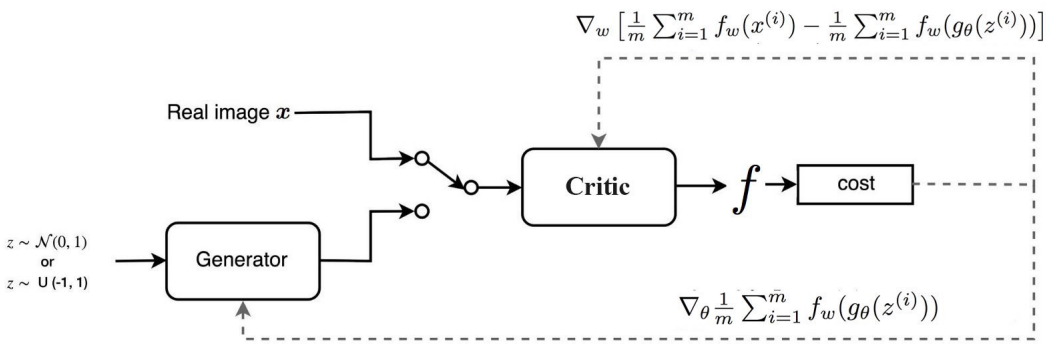


Figure 25.5: WGAN

	Discriminator/Critic	Generator
GAN	$\nabla_{\theta_d} \frac{1}{m}\sum_{i=1}^m \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)\right]$	$\nabla_{\theta_g} \frac{1}{m}\sum_{i=1}^m \log\left(D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)$
WGAN	$\nabla_w \frac{1}{m}\sum_{i=1}^m \left[f(x^{(i)}) - f(G(z^{(i)}))\right]$	$\nabla_\theta \frac{1}{m}\sum_{i=1}^m f(G(z^{(i)}))$

Figure 25.6: WGAN

25.5 InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets

25.5.1 Joint Entropy

$$H(X,Y) = \mathbb{E}_{X,Y}[-\log p(x,y)] = -\sum_{x,y} p(x,y)\log p(x,y)$$

25.5.2 Conditional Entropy

$$\begin{aligned}
H(X|Y) &= \mathbb{E}_Y[H(X,Y)] \\
&= -\sum_{y\sim p_Y(y)} p(y) \sum_{x\sim p_X(x)} p(x|y)\log p(x|y) \\
&= -\sum_{y\sim p_Y(y)} \sum_{x\sim p_X(x)} p(y)p(x|y)\log p(x|y) \\
&= -\sum_{y\sim p_Y(y)} \sum_{x\sim p_X(x)} p(x,y)\log p(x|y) = -\mathbb{E}_{x,y}[\log p(x|y)] \\
&= -\sum_{y\sim p_Y(y)} \sum_{x\sim p_X(x)} p(x,y)\log \frac{p(x,y)}{p(y)} \\
&= -\sum_{y\sim p_Y(y)} \sum_{x\sim p_X(x)} p(x,y)\log p(x,y) + \sum_{y\sim p_Y(y)} \sum_{x\sim p_X(x)} p(x,y)\log p(y) \\
&= H(X,Y) - H(Y)
\end{aligned}$$

25.5.3 Variational Mutual Information Maximization

$$\begin{aligned}
I(c;G(z,c)) &= H(c) - H(c|G(z,c)) \\
&= H(c) + \int\int p(c=c', x=G(z,c))\log p(c=c'|x=G(z,c))dc'dz \\
&= H(c) + \mathbb{E}_{x\sim G(z,c),c'\sim p(c|x)}[\log p(c'|x)] \\
&= H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}[\log p(c'|x)] \\
&= H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\left[\log \frac{p(c'|x)Q(c'|x)}{Q(c'|x)}\right] \\
&= H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\left[\log \frac{p(c'|x)}{Q(c'|x)}\right] + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big] \\
&= H(c) + \mathbb{E}_{x\sim G(z,c)}\Big[D_{KL}(p(c'|x)||Q(c'|x))\Big] + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big] \\
&\geq H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big]^{2}
\end{aligned}$$

Thus we get a lower bound for the mutual information as follows:

$$I(c; G(z,c)) \geq H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big]$$

However, we still have a problem. We need to sample c from $p(c|x)$. Thus, we need to replace it with a known distribution. Firstly, with the reasoning that $x \sim G(z,c)$ means sample c from $p(c)$ then sample x from $G(z,c)$. So we can express $\mathbb{E}_{x\sim G(z,c)}$ with $\mathbb{E}_{c\sim p(c)}\mathbb{E}_{x\sim G(z,c)}$. and by the Lemma 1,

$$\begin{aligned} I(c; G(z,c)) &\geq H(c) + \mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big] \\ &= H(c) + \mathbb{E}_{c\sim p(c)}\mathbb{E}_{x\sim G(z,c)}\mathbb{E}_{c'\sim p(c|x)}\Big[\log Q(c'|x)\Big] \\ &= H(c) + \mathbb{E}_{c\sim p(c)}\mathbb{E}_{x\sim G(z,c)}\Big[\log Q(c'|x)\Big]^{3} \end{aligned}$$

Thus, we can directly sample c from the known distribution instead of $p(c|x)$.

lemma 1 *For random variables X, Y and function $f(x,y)$ under suitable regularity conditions:*

$$\mathbb{E}_{x\sim X, y\sim Y|x}[f(x,y)] = \mathbb{E}_{x\sim X, y\sim Y|x, x'\sim X|y}[f(x',y)]$$

proof 1

$$\begin{aligned} \mathbb{E}_{x\sim X, y\sim Y|x}[f(x,y)] &= \int_x P(x)\int_y P(y|x)f(x,y)dydx \\ &= \int_x\int_y P(x,y)f(x,y)dydx \\ &= \int_{x'}\int_y P(x',y)f(x',y)dydx' \\ &= \int_{x'}\int_y P(y)P(x'|y)f(x',y)dydx' \\ &= \int_{x'}\int_y\int_x P(x,y)P(x'|y)f(x',y)dxdydx' \\ &= \int_x P(x)\int_y P(x|y)\int_{x'} P(x'|y)f(x',y)dxdydx' \\ &= \mathbb{E}_{x\sim X, y\sim Y|x, x'\sim X|y}[f(x',y)] \end{aligned}$$

Chapter 26

Diffusion Model

26.1 Introduction

(Denoising) Diffusion models have emerged as the new SOTA family of deep generative models.

- First proposed in 2015.
- Outperform GANs on image synthesis (DDPM) $\sim$ 2020.
- Stable training dynamics.
- Image synthesis, super resolution, text-to-image, and so on.

The overall idea is to construct a Markov chain of progressively less noisy samples. Each transition denoises a noisy sample. Diffusion models consist of two Markov chains:

1. Forward: A Markov chain of diffusion steps to **slowly add random noise** to data.

$$\underbrace{\mathbf{x}_0}_{\text{data}} \to \mathbf{x}_1 \cdots \to \underbrace{\mathbf{x}_T}_{\text{noise}}$$

   - $\mathcal{D}_{data} \to \mathcal{N}$.

2. Backward (Reverse): Learn to **reverse the diffusion process** to construct desired data samples from the noise.

$$\underbrace{\mathbf{x}_T}_{\text{noise}} \to \mathbf{x}_{T-1} \cdots \to \underbrace{\mathbf{x}_0}_{\text{data}}$$

   - $\mathcal{N} \to \mathcal{D}_{data}$.

Breaking the overall process into smaller steps allows us to use simple distributions at each step. As will be discussed in the following subsections, we can use Gaussian distributions for the transitions. Thanks to the properties of a Gaussian, the posterior will remain a Gaussian if the likelihood and the prior are both Gaussians. Therefore, if each transitional distribution above is a Gaussian, the joint distribution is also a Gaussian. Since a Gaussian is fully characterized by the first two moments (mean and variance), the computation is highly tractable.

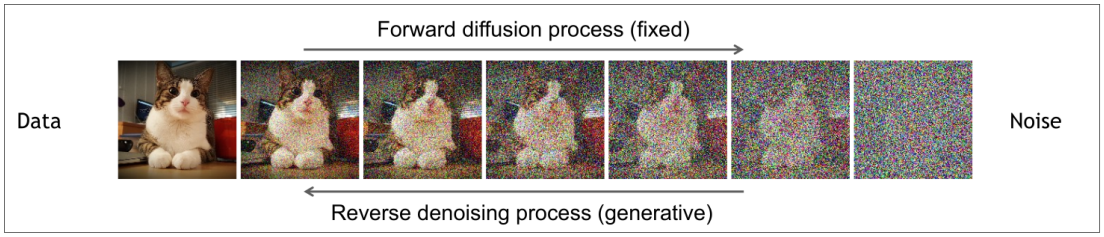


Figure 26.1: CVRP 2022 Tutorial: Denoising Diffusion-based Generative Modeling: Foundations and Applications

This particular structure is called the *variational diffusion model*.

Some properties of diffusion models:

1. Diffusion model has a pre-defined sampling equation.
    - The equation relies on a random noise.
    - Noise is all we need $\rightarrow$ Predict noise at a time step t.
2. Fit a model via forward and backward processes.
3. **Iterative transform** of one distribution into another via **Makov Chain**.
    - Diffusion model$\approx$Generative Markov Chain.
4. We want to learn a transition model:
$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}|\boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)).$$
5. Base case: $p(\mathbf{x}_T) = \mathcal{N}(0, I)$
6. Marginal distribution over $\mathbf{x}_0$ can be expressed as follows:
$$p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_0, \ldots, \mathbf{x}_T) d\mathbf{x}_1, \ldots, \mathbf{x}_T$$
    - Similar to the VAE, the $\mathbf{x}_1, \ldots, \mathbf{x}_T$ can be considered as latent variables, since we don't know.
7. The goal is to learn the parameters so that
$$p(\mathbf{x}_0) \approx p_\theta(\mathbf{x}_0)$$

26.2 Forward Diffusion

Let's first model a forward trajectory by using the *Markov property*:

$$q(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} \underbrace{q(\mathbf{x}_t|\mathbf{x}_{t-1})}_{\text{Transition kernel}}$$

- *Slow transform with a large T*: $\mathbf{x}_0 \to \mathbf{x}_1 \cdots \to \mathbf{x}_T$
  - To track the transitions of data, we will try to model as many steps as possible.
- The question is how to model $q(\mathbf{x}_t|\mathbf{x}_{t-1})$?

In a continuous case (*e.g.,* image), forward diffusion $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ can be parameterized as follows:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \tag{26.1}$$

- $\beta_t \in (0, 1)$ is a variance at time t.
- $\sqrt{1-\beta_t}$ downscales $\mathbf{x}_{t-1}$ to be 0, $\beta_1 < \cdots < \beta_t$. Thus, $\mathbf{x}_t$ will become more noisier than $\mathbf{x}_{t-1}$. Then, $\mathbf{x}_t$ can be sampled as:

$$\mathbf{x}_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t} \odot \epsilon$$

  1. Sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ and scale it by $\sqrt{1-\beta_t}$
  2. Adds noise $\epsilon \sim \mathcal{N}(0, I)$ with variance β_t.
- The above process is autoregressive (*i.e.,* ancestral sampling), but we can sample $\mathbf{x}_t$ directly from $q(\mathbf{x}_t|\mathbf{x}_0)$ in an analytic form:

$$\begin{aligned}
\mathbf{x}_t &= \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t} \odot \epsilon_{t-1} && (26.2)\\
&= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t} \odot \epsilon_{t-1} && (26.3)\\
&= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_{t-1}} \odot \epsilon_{t-2}\right) + \sqrt{1-\alpha_t} \odot \epsilon_{t-1} && (26.4)\\
&= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t\alpha_{t-1}} \odot \epsilon_{t-2} + \sqrt{1-\alpha_t} \odot \epsilon_{t-1} && (26.5)\\
&= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t\alpha_{t-1} + 1 - \alpha_t} \odot \epsilon_{t-2} && (26.6)\\
&= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1 - \alpha_t\alpha_{t-1}} \odot \epsilon_{t-2} && (26.7)\\
&= \dots && (26.8)\\
&= \sqrt{\prod_t \alpha_t}\mathbf{x}_0 + \sqrt{1 - \prod_t \alpha_t} \odot \epsilon_{t_0} && (26.9)\\
&= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t} \odot \epsilon && (26.10)\\
&\sim \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}), && (26.11)
\end{aligned}$$

  where $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$. Thus, $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t} \odot \epsilon$. Note that the fifth step is done by using the property of sum of two Gaussian distributions (*e.g.,* $\mathcal{N}(0, \sigma_1^2 I) + \mathcal{N}(0, \sigma_2^2 I) = \mathcal{N}(0, (\sigma_1^2 + \sigma_2^2)I)$).

We can get some intuitions:

- The original input $\mathbf{x}_0$ **gradually loses all info** during the forward diffusion process.
- This Markov chain has a **stationary distribution** *i.e.,* as $t \to \infty$, $q(\mathbf{x}_t) \approx \mathcal{N}(0, I)$.
  - In practice, T is set to be a very high number *e.g.,* 1,000.
  - The high T minimizes the information loss at each step, which allows a smooth training.
- The forward diffusion process does not require any training.

26.3 Backward Process

In the forward process, we model the diffusion process, which turns the input data into the noisy data. However, a noisy data is not what we want to obtain. What we want is to generate a new data with high quality.

To generate data, we will reverse the forward process. Then, we can reconstruct the true data. We call this process *Backward process*! The backward process works as follows:

- Start from the noise distribution $q(\mathbf{x}_T) \approx \mathcal{N}(0, I)$.
- Then, sample a noise $\mathbf{x}_T \sim \mathcal{N}(\mathbf{x}_T|0, I)$
- Iteratively sample $\mathbf{x}_{t-1} \sim q(\mathbf{x}_{t-1}|\mathbf{x}_t)$.
  - Note that $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is the **true denoising distribution** that we have no access.
  - In general, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is intractable.
- We can **approximate** $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ as **Normal distribution** if β_t is small enough in each forward diffusion step.
- We will approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ using a neural network, $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$.
- $p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$.
  - $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; 0, I)$.
  - $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$.
  - We can model the denoising distribution as Normal distribution like above (*c.f.*, Eq. (26.35)).
  - Note that the reverse conditional probability $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is tractable when it is conditioned on $\mathbf{x}_0$ as shown in Eq. (26.35). This allows us to train a neural network to model this denoising distribution.
- Key to the success of this sampling process is training the reverse Markov chain to match the actual time reversal of the forward Markov chain.
- After optimizing the backward process, the sampling procedure is that just sample Gaussian noise from $p(\mathbf{x}_T)$ and then iteratively running the denoising transitions (backward process) for T steps to generate a novel $\mathbf{x}_0$.

26.4 Distribution Modeling

What we want to learn (or model) is $p_\theta(\mathbf{x}_0) \approx p(\mathbf{x}_0)$ (approximate data distribution).

- $p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T}$
- It is intractable to compute all trajectories (*i.e.,* integral over all $\mathbf{x}_{1:T}$).
- Thus, we will deviate the issue by leveraging a variational lower bound with KL-Divergence as follows:

The log-likelihood of p_θ is given by

$$\begin{aligned}
\log p_\theta(\mathbf{x}_0) &= \log \int p(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} && (26.12)\\
&= \log \int p(\mathbf{x}_{0:T}) \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} d\mathbf{x}_{1:T} && (26.13)\\
&= \log \int q(\mathbf{x}_{1:T}|\mathbf{x}_0) \frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} d\mathbf{x}_{1:T} && (26.14)\\
&\geq \int q(\mathbf{x}_{1:T}|\mathbf{x}_0) \log \frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} d\mathbf{x}_{1:T} \quad \text{by Jensen's Inequality} && (26.15)\\
&= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log \frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right] \quad (\textbf{ELBO}) && (26.16)\\
&= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log p(\mathbf{x}_T) \prod_{t=1}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right] \quad \text{by Markov Property} && (26.17)\\
&= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log \frac{p(\mathbf{x}_T) p(\mathbf{x}_0|\mathbf{x}_1) \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_T|\mathbf{x}_{T-1}) \prod_{t=1}^{T-1} q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right] && (26.18)\\
&= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log \frac{p(\mathbf{x}_T) p(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_T|\mathbf{x}_{T-1})} \right] + \underbrace{\mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log \prod_{t=1}^{T-1} \frac{p(\mathbf{x}_t|\mathbf{x}_{t+1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right]}_{\text{Consistency term}} && (26.19)
\end{aligned}$$

The first term of the last line can be further decomposed:

$$\underbrace{\mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)]}_{\text{Reconstruction}} + \underbrace{\mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_{T-1})} \right]}_{\text{Prior matching}} + \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[\sum_{t=1}^{T-1} \log \frac{p(\mathbf{x}_t|\mathbf{x}_{t+1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right]$$

The *reconstruction term* can be simplified as follows:

$$\mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)].$$

This is because we can ignore the steps $[2, \ldots, T]$, which are unrelated to the calculation of the expectation.

The *prior matching term* ensures that the latent distribution at the end of the diffusion step is similar to a prior distribution, which is a Gaussian distribution. Note that the *prior matching term* requires no optimization, as it has no trainable parameters. Recall that we have assumed a large enough T such that the final distribution is Gaussian, this term effectively becomes zero.

Now, let's simplify the prior matching term. First, we will only consider the $\mathbf{x}_T, \mathbf{x}_{T-1}$ since the conditional probability depends only on them. Then, the expectation term $q(\mathbf{x}_{1:T}|\mathbf{x}_0)$ becomes:

$$\begin{aligned} q(\mathbf{x}_{1:T}|\mathbf{x}_0) &= q(\mathbf{x}_T, \mathbf{x}_{T-1}|\mathbf{x}_0) \\ &= q(\mathbf{x}_T, \mathbf{x}_{T-1}, \mathbf{x}_0)/q(\mathbf{x}_0) \\ &= q(\mathbf{x}_{T-1}|\mathbf{x}_0)q(\mathbf{x}_T|\mathbf{x}_{T-1}, \mathbf{x}_0) \quad \text{by Chain Rule} \\ &= q(\mathbf{x}_{T-1}|\mathbf{x}_0)q(\mathbf{x}_T|\mathbf{x}_{T-1}) \quad \text{by Markov Property} \end{aligned}$$

By using the above simplification,

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_{T-1})}\right] &= \mathbb{E}_{q(\mathbf{x}_{T-1}|\mathbf{x}_0)}\left[\mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_{T-1})} \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_{T-1})}\right] \\ &= -\mathbb{E}_{q(\mathbf{x}_{T-1}|\mathbf{x}_0)}\left[D_{KL}[q(\mathbf{x}_T|\mathbf{x}_{T-1})\|p(\mathbf{x}_T)]\right]. \end{aligned}$$

Finally, the *consistency term* can be expressed as follows:

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\sum_{t=1}^{T-1} \log \frac{p(\mathbf{x}_t|\mathbf{x}_{t+1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] &= \sum_{t=1}^{T-1} \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_t, \mathbf{x}_{t+1}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_t|\mathbf{x}_{t+1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \\ &= -\sum_{t=1}^{T-1} \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_{t+1}|\mathbf{x}_0)}\left[D_{KL}[q(\mathbf{x}_t|\mathbf{x}_{t-1})\|p(\mathbf{x}_t|\mathbf{x}_{t+1})]\right] \end{aligned}$$

Note that the last step is done by the chain rule:

$$q(\mathbf{x}_t, \mathbf{x}_{t-1}|\mathbf{x}_0) = \frac{q(\mathbf{x}_t, \mathbf{x}_{t-1}, \mathbf{x}_0)}{q(\mathbf{x}_0)} = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}, \mathbf{x}_0)}{q(\mathbf{x}_0)} = q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1}|\mathbf{x}_0)$$

In sum, we derive the ELBO and its factorized form is given by

$$\begin{aligned} \log p_\theta(\mathbf{x}_0) &\geq \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \\ &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] - \mathbb{E}_{q(\mathbf{x}_{T-1}|\mathbf{x}_0)}\left[D_{KL}[q(\mathbf{x}_T|\mathbf{x}_{T-1})\|p(\mathbf{x}_T)]\right] \\ &\quad - \sum_{t=1}^{T-1} \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_{t+1}|\mathbf{x}_0)}\left[D_{KL}[q(\mathbf{x}_t|\mathbf{x}_{t-1})\|p(\mathbf{x}_t|\mathbf{x}_{t+1})]\right]. \end{aligned}$$

Let's closely look at the consistency term.

- It endeavors to make the distribution at x_t consistent, from both forward and backward processes. That is, a denoising step from a noisier image should match the corresponding noising step from a cleaner image, for every intermediate timestep. This term is minimized when we train $p_\theta(\mathbf{x}_t|\mathbf{x}_{t+1})$ to match the Gaussian distribution $q(\mathbf{x}_t|\mathbf{x}_{t-1})$, which is defined in Eq. (26.1).

- Under this derivation, all terms of the ELBO are computed as expectations, and can therefore be approximated using Monte Carlo estimates.

- The challenge of the above variational diffusion model is that we need to draw samples (x_{t-1}, x_{t+1}) from a joint distribution $q(x_{t-1}, x_{t+1}|x_0)$ for every time step t. Thus, the variance of its Monte Carlo estimate could potentially be higher than a term that is estimated using only one random variable per time step. As it is computed by summing up $T-1$ consistency terms, the final estimated value of the ELBO may have high variance for large T values.

Let us instead try to derive a new ELBO, where each term is computed as an expectation over one random variable at a time. The key insight is that we can rewrite encoder transitions as $q(x_t|x_{t-1}) = q(x_t|x_{t-1}, x_0)$, where the extra conditioning term is superfluous due to the Markov property. Then, according to Bayes rule, we can rewrite each transition as:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}.$$

Armed with this equation, we can factorize the ELBO again as follows:

$$L = \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \quad \rightarrow \text{ELBO} \tag{26.20}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log p(\mathbf{x}_T) \prod_{t=1}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \tag{26.21}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)\prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_1|\mathbf{x}_0)\prod_{t=2}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \tag{26.22}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)\prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_1|\mathbf{x}_0)\prod_{t=2}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)}\right] \quad \text{by Markov Property} \tag{26.23}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)} + \log \prod_{t=2}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)}\right] \tag{26.24}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)} + \log \prod_{t=2}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}}\right] \tag{26.25}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)} + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \log \prod_{t=2}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)}\right] \tag{26.26}$$

$$= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)p(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \log \prod_{t=2}^{T} \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)}\right] \tag{26.27}$$

$$= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] + \mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)}\right] \tag{26.28}$$

$$+ \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_t, \mathbf{x}_{t-1}|\mathbf{x}_0)}\left[\log \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)}\right] \tag{26.29}$$

$$= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] - D_{KL}(q(\mathbf{x}_T|\mathbf{x}_0)||p(\mathbf{x}_T)) \tag{26.30}$$

$$- \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}[D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p(\mathbf{x}_{t-1}|\mathbf{x}_t))] \tag{26.31}$$

Let's delve into the last three terms:

- $\mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)]$: Reconstruction term.
- $D_{KL}[q(\mathbf{x}_T|\mathbf{x}_0)||p(\mathbf{x}_T)]$: Prior matching term.
  - No trainable parameters, since it can be fully characterized by $\mathbf{x}_t$ and $\mathbf{x}_0$, so we don't need a neural network to estimate it.
- $\sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}[D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p(\mathbf{x}_{t-1}|\mathbf{x}_t))]$: Consistency term (or denoising matching term).

We can notice that the consistency term requires to estimate three different probabilities:

1. $q(\mathbf{x}_t|\mathbf{x}_0)$: we can sample $\mathbf{x}_t$ by only using $\mathbf{x}_0$ and ϵ as we derived before:
$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t} \odot \epsilon$$
2. $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$: This distribution says we want to sample a less noisy sample $\mathbf{x}_{t-1}$ using the clean sample $\mathbf{x}_0$ and its noisy version $\mathbf{x}_t$. In other words, we want to denoise the sample by using the two samples.
3. $p(\mathbf{x}_{t-1}|\mathbf{x}_t)$: We are going to use a distribution parameterized by θ, which is a neural network. We can rewrite this as follows:
$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

In sum, the consistency term or denoising matching term is the term for training a neural network to make it learn how to denoise samples. Let's compute the KL divergence:

By using the chain rule, $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ can be factorized as follows:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)}.$$

Then, $q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) = q(\mathbf{x}_t|\mathbf{x}_{t-1})$ by Markov property. Then we get

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \tag{26.32}$$

$$= \frac{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_{t-1}, (1-\bar{\alpha}_t)\mathbf{I})\mathcal{N}(\mathbf{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0, (1-\bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})} \tag{26.33}$$

$$\vdots \tag{26.34}$$

$$\propto \mathcal{N}\Bigg(\mathbf{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\mathbf{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\mathbf{x}_t, \mathbf{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\Sigma_q(t)}\Bigg), \tag{26.35}$$

where $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$. We have shown that at each step, $\mathbf{x}_{t-1} \sim q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ is still normally distributed, with mean $\mu_q(\mathbf{x}_t, \mathbf{x}_0)$ that is a function of $\mathbf{x}_t$ and $\mathbf{x}_0$, and variance $\Sigma_q(t)$ as a function of α coefficients. We can rewrite the variance as $\Sigma_q(t) = \sigma_q^2(t)\mathbf{I}$.

We can also notice that the mean $\boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ is a linear combination of $\mathbf{x}_t$ and $\mathbf{x}_0$. Geometrically, it lives on the straight line connecting $\mathbf{x}_t$ and $\mathbf{x}_0$. In other words, the denoised sample $\mathbf{x}_{t-1}$ stays somewhere between the $\mathbf{x}_t$ and $\mathbf{x}_0$.

Another observation is that the coefficient of $\mathbf{x}_t$ increases and that of $\mathbf{x}_0$ decreases. Conversely, $\mathbf{x}_t$ decreases and that of $\mathbf{x}_0$ increases as t goes to 0 from T.

In order to match approximate denoising transition step $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ to the denoising transition step $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ as closely as possible, we can also model it as a Gaussian. Let's simplify the KL divergence:

$$\begin{aligned}
&D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) \\
&= D_{KL}(\mathcal{N}(\mathbf{x}_{t-1}; \mu_q, \Sigma_q(t))\|\mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta, \Sigma_q(t))) \\
&\vdots \\
&= \frac{1}{2\sigma_q^2(t)}\|\boldsymbol{\mu}_\theta(\mathbf{x}_t) - \boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)\|_2^2.
\end{aligned}$$

By using this, we can rewrite the ELBO that we want to maximize:

$$\text{ELBO}_\theta(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] - \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[\frac{1}{2\sigma_q^2(t)} \|\boldsymbol{\mu}_\theta(\mathbf{x}_t) - \boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)\|_2^2 \right]$$

Note that the reconstruction term can be analytically computed, so we can make simplify further.

26.5 Training and Inference

Recall that the ELBO we derived suggests that we need to minimize the following equation:

$$\frac{1}{2\sigma_q^2(t)}\|\boldsymbol{\mu}_\theta(\mathbf{x}_t) - \boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)\|_2^2$$

We already know that $\boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ is given by

$$\boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\mathbf{x}_0}{1-\bar{\alpha}_t}.$$

Therefore, $\boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ can be fully characterized by $\mathbf{x}_t$ and $\mathbf{x}_0$.

Next, we need to design $\boldsymbol{\mu}_\theta$ and we can set it to follow a simple form, which is similar to $\boldsymbol{\mu}_q$. Then, we get

$$\boldsymbol{\mu}_\theta(\mathbf{x}_t) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\hat{\mathbf{x}}_\theta(\mathbf{x}_t)}{1-\bar{\alpha}_t},$$

where $\hat{\mathbf{x}}_\theta$ is another network that seeks to predict $\mathbf{x}_0$ from noisy image $\mathbf{x}_t$ at t-th step. Then, the KL divergence becomes

$$\frac{1}{2\sigma_q^2(t)}\|\boldsymbol{\mu}_\theta(\mathbf{x}_t) - \boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)\|_2^2 = \frac{1}{2\sigma_q^2(t)}\frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2}\|\hat{\mathbf{x}}_\theta(\mathbf{x}_t) - \mathbf{x}_0\|_2^2$$

This indicates that optimizing a VDM boils down to learning a neural network to predict the original ground truth sample from an arbitrarily noisy version of it.

Finally, we get

$$\text{ELBO}_\theta(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p(\mathbf{x}_0|\mathbf{x}_1)] - \sum_{t=2}^{T}\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left[\frac{1}{2\sigma_q^2(t)}\frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2}\|\hat{\mathbf{x}}_\theta(\mathbf{x}_t) - \mathbf{x}_0\|_2^2\right].$$

This implies that optimizing VDM is equivalent to a denoising problem as we need to find a network $\hat{\mathbf{x}}_\theta(\mathbf{x}_t)$ such that $\mathbf{x}_t$ will be close to the ground truth $\mathbf{x}_0$.

- We are not going to predict arbitrary noisy samples.
- The noisy sample $\mathbf{x}_t$ is carefully crafted by the forward sampling equation.

26.6 Noise Prediction

$$\mathbf{x}_0 = \frac{\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}}$$

By plugging the above equation, we get:

$$\boldsymbol{\mu}_\theta(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}}\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\mathbf{x}_t)$$

$$\begin{aligned} & D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p(\mathbf{x}_{t-1}|\mathbf{x}_t)) \\ & \quad \vdots \\ & \quad = \frac{1}{2\sigma_q^2(t)} \frac{(1-\alpha_t)^2}{(1-\bar{\alpha}_t)\alpha_t} \left[\|\hat{\boldsymbol{\epsilon}}_\theta(\mathbf{x}_t) - \boldsymbol{\epsilon}_0\|_2^2 \right]. \end{aligned}$$

The $\hat{\boldsymbol{\epsilon}}_\theta(\mathbf{x}_t)$ is a neural network that learns to predict the source noise $\boldsymbol{\epsilon}_0 \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \mathbf{I})$. This indicates that learning a VDM by predicting the original image $\mathbf{x}_0$ is equivalent to learning to predict the noise; empirically, however, some works have found that predicting the noise resulted in better performance.

26.7 Summary

- The loss function can be decomposed.

$$L_{\text{VLB}} = L_T + L_{T-1} + \cdots + L_0.$$

- $L_T = D_{\text{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_\theta(\mathbf{x}_T))$
  - Constant ≈ 0 since x_T is a Gaussian noise.
- $L_t = D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))$ for $t > 1$
  - This is the main part.
- $L_0 = -\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)$
  - Can be modeled by a separate decoder.
- $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)I)$
- $q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$,

  We can sample by $\mathbf{x}_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t}\epsilon$
- $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$.
  - We need to learn mean and variance.
  - DDPM kept the variance fixed and let the neural network only learn the mean μ_θ.
  - $\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) = \sigma_t^2\mathbf{I}$ and set $\sigma_t^2 = \beta_t$.
  - Improved DDPM model trains σ also.
- One can reparameterize the mean to make the nerual network learn the added noise via a network ϵ_θ.

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\underbrace{\epsilon_\theta(\mathbf{x}_t, t)}_{\text{Network}}\right)$$

- Final objective function L_t is

$$||\epsilon - \epsilon_\theta(\mathbf{x}_t, t)||^2 = ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon, t)||^2$$

  - $t \sim \text{Unif}[\{1, .., T\}]$
  - $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon \sim q(\mathbf{x}_t|\mathbf{x}_0)$
  - $\epsilon \sim \mathcal{N}(0, I)$
- $\mathbf{x}_t$ is perturbed by ϵ and the noise prediction network ϵ_θ predicts ϵ.

Algorithm 6: Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \text{Unif}[\{1, \cdots, T\}]$
  $\epsilon \sim \mathcal{N}(0, I)$
  Take gradient descent step on $\nabla_\theta ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon, t)||^2$
until *converged*;

The training process is given by

1. $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
2. Sample a noise level t between 1 and T (*i.e.,* random time step).
3. Sample a noise from a Gaussian distribution and perturb the input by the sampling equation.
4. NN is trained to predict this noise ϵ used for generating $\mathbf{x}_t$.
5. β is often scheduled linearly.
6. Σ is set equal to β.

The sampling process is given by

Algorithm 7: Sampling

$\mathbf{x}_T \sim \mathcal{N}(0, I)$
for $t = T, \cdots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(0, I)$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \Sigma_t \mathbf{z}$
return $\mathbf{x}_0$

- Ancestral sampling.
- T is typically around 1,000

26.8 Score Matching

- Suppose $\{\mathbf{x}_0, \cdots, \mathbf{x}_N\}$, where each data point (*e.g.,* image, video, or text)) is sampled independently from a data distribution $p(\mathbf{x})$.
- Given the dataset, the goal of generative modeling is to fit a model to the data distribution such that we can synthesize new data points at will by sampling from the model.
- One way is to directly model the distribution function as in likelihood-based models. Let $f_\theta(\mathbf{x}) \in \mathbb{R}^d$, then we can define a density function:

$$p_\theta(\mathbf{x}) = \frac{\exp^{-f_\theta(\mathbf{x})}}{Z_\theta}$$

.

- $f_\theta(\mathbf{x}) \in \mathbb{R}^d$ is often called unnormalized probabilistic model or energy-based model.
- Energy-based model originates from the Gibbs distribution in statistical physics.
- $p_\theta(\mathbf{x})$ can be trained by maximizing the log-likelihood of the data.

$$\max_\theta \sum_i^N \log p_\theta(\mathbf{x}_i).$$

- The gradient of the loglikelihood is given by

$$\begin{aligned}
\nabla_\theta \log p_\theta(\mathbf{x}) &= \nabla_\theta f_\theta(\mathbf{x}) - \nabla_\theta Z_\theta \\
\nabla_\theta Z_\theta &= \frac{\nabla_\theta Z_\theta}{Z_\theta} \\
&= \frac{1}{Z_\theta} \nabla_\theta \int \exp(f_\theta(\mathbf{x})) d\mathbf{x} \\
&= \frac{1}{Z_\theta} \int \exp(f_\theta(\mathbf{x})) \nabla_\theta f_\theta(\mathbf{x}) d\mathbf{x} \\
&= \int \frac{1}{Z_\theta} \exp(f_\theta(\mathbf{x})) \nabla_\theta f_\theta(\mathbf{x}) d\mathbf{x} \\
&= \int p_\theta(\mathbf{x}) \nabla_\theta f_\theta(\mathbf{x}) d\mathbf{x} \\
&= \mathbb{E}_{p_\theta(\mathbf{x})}[\nabla_\theta f_\theta(\mathbf{x})] \\
\nabla_\theta \log p_\theta(\mathbf{x}) &= \nabla_\theta f_\theta(\mathbf{x}) - \mathbb{E}_{p_\theta(\mathbf{x})}[\nabla_\theta f_\theta(\mathbf{x})]
\end{aligned}$$

- However, it is undesirable, since Z_θ is intractable.
  - For instance, a gray scale image of 100×100 has $256^{10,000}$ space.
- Thus, we have to sidestep the issue by using some solutions, for instance:
  - Approximate by using VAE or MCMC

Instead, we can leverage ***Stein Score***:

- By modeling a score function, instead of the density function, we can sidestep the difficulty of computing the intractable normalizaing constants.

- *Stein Score* function: $\nabla_{\mathbf{x}} \log p(\mathbf{x})$.
  - **Not a gradient w.r.t. model parameters.**
  - Gradient of the log probability density function.
  - Not same as the score in stat.
- It is a direction that maximizes a log data density.
- A model for approximating the score function is called a *score-based model* $s_\theta(\mathbf{a})$.
- Score-based models does not have to compute the intractable normalizing constant, Z_θ.

$$s_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) = -\nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \underbrace{\nabla_{\mathbf{x}} \log Z_\theta}_{\text{Constant}}.$$

26.8.1 Fisher Divergence

We need to know about *Fisher Divergence*:

- Given *i.i.d.* samples $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\} \sim p_{data}(\mathbf{x}) = p(\mathbf{x})$.
- Estimating the score function $\nabla_{\mathbf{x}} \log p(\mathbf{x})$.
- Score model $s_\theta(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^D$.
- Use score estimator $s_\theta(x)$:

$$\mathcal{L}_\theta = \frac{1}{2}\mathbb{E}_{p(\mathbf{x})}\left[||\nabla_{\mathbf{x}} \log p(\mathbf{x}) - s_\theta(\mathbf{x})||_2^2\right].$$

- It is called *Fisher divergence*.
- Intuitively, the Fisher divergence compares the squared distance between the ground-truth data score and the score-based model.
  - It changes the problem into a *regression* problem.
- Direct computation of the divergence is **infeasible** due to the unknown data score $\nabla_{\mathbf{x}} \log p(\mathbf{x})$.
  - Since we have no access to the true data distribution $p(\mathbf{x})$.

Fortunately, there exists a family of methods called ***score matching*** that minimize the Fisher divergence without knowledge of the ground-truth data score.

- Score matching objectives can directly be estimated on a dataset and optimized with stochastic gradient descent, analogous to the log-likelihood objective for training likelihood-based models (with known normalizing constants).
- We can train the score-based model by minimizing a score matching objective, without requiring adversarial optimization.

$$\mathcal{L}_\theta = \mathbb{E}_{p(\mathbf{x})}\left[\frac{1}{2}||s_\theta(x)||_2^2 + tr(\nabla_{\mathbf{x}} s_\theta(x))\right]$$
$$\approx \frac{1}{N}\sum_{i=1}^{N}\left[\frac{1}{2}||s_\theta(x)||_2^2 + tr(\nabla_{\mathbf{x}} s_\theta(x))\right]$$

- $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\} \sim p(\mathbf{x})$
- $\nabla_{\mathbf{x}} s_\theta(x)$: Jacobian
- Remove the dependency of $p(\mathbf{x})$

$$\mathcal{L}_\theta = \frac{1}{2}\mathbb{E}_{p(x)}\left[||\nabla_x \log p(x) - s_\theta(x)||_2^2\right] \tag{26.36}$$
$$= \frac{1}{2}\mathbb{E}_{p(x)}\left[\left(\nabla_x \log p(x) - s_\theta(x)\right)^2\right] \tag{26.37}$$
$$= \frac{1}{2}\int p(x)(\nabla_x \log p(x) - s_\theta(x))^2 dx \tag{26.38}$$
$$= \underbrace{\frac{1}{2}\int p(x)(\nabla_x \log p(x))^2 dx}_{\text{independent from theta}} + \frac{1}{2}\int p(x) s_\theta(x)^2 dx - \int p(x) s_\theta(x) \nabla_x \log p(x) dx \tag{26.39}$$
$$= \cdots - \int p(x) s_\theta(x) \nabla_x \log p(x) dx \tag{26.40}$$
$$= \cdots - \int p(x) s_\theta(x) \frac{\nabla_x p(\mathbf{x})}{p(x)} dx \tag{26.41}$$
$$= \cdots - \int \nabla_{\mathbf{x}} p(x) s_\theta(x) dx \tag{26.42}$$
$$= \cdots - \left[p(x) s_\theta(x)\right]_{x=-\infty}^{\infty} + \int p(x) \nabla_x s_\theta(x) dx \tag{26.43}$$
$$= \frac{1}{2}\int p(x) s_\theta(x)^2 dx + \int p(x) \nabla_x s_\theta(x) dx + \text{const} \tag{26.44}$$
$$= \frac{1}{2}\mathbb{E}_{p(x)}[s_\theta(x)^2] + \mathbb{E}_{p(x)}[\nabla_x s_\theta(x)] + \text{const.} \tag{26.45}$$

- The second last term used the integration by parts.
- The last step is done by a boundary condition assumption which makes score function to be zero (*c.f.,* Sliced score matching paper).
  - $p_{data}(x) \to 0$ as $|x| \to \infty$.
  - In other words, gradient vanishes on the boundary.

26.8.2 Langevin Dynamics

- Once we have trained a score-based model $s_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$, we can use an iterative procedure called *Langevin Dynamics* (LD) [**?**] to draw samples from it.
- LD provides an MCMC procedure to sample from a distribution $p(\mathbf{x})$ using only its score function.

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} + \frac{\epsilon}{2}\nabla_{\mathbf{x}} \log p(\mathbf{x}_{t-1}) + \sqrt{\epsilon}\mathbf{z}_t$$

- Specifically, it initializes the chain from an arbitrary prior distribution $\mathbf{x}_0 \sim \pi(\mathbf{x})$, and then iterates the following
- Sample from $p(x)$ using only the score $\nabla_x \log p(x)$.
- $\mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.
- ϵ is the step size.
- As $T \to \infty$ and $\epsilon \to 0$, $\mathbf{x}_T$ will become the true probability density $p(\mathbf{x})$.

Chapter 27

Flow Models

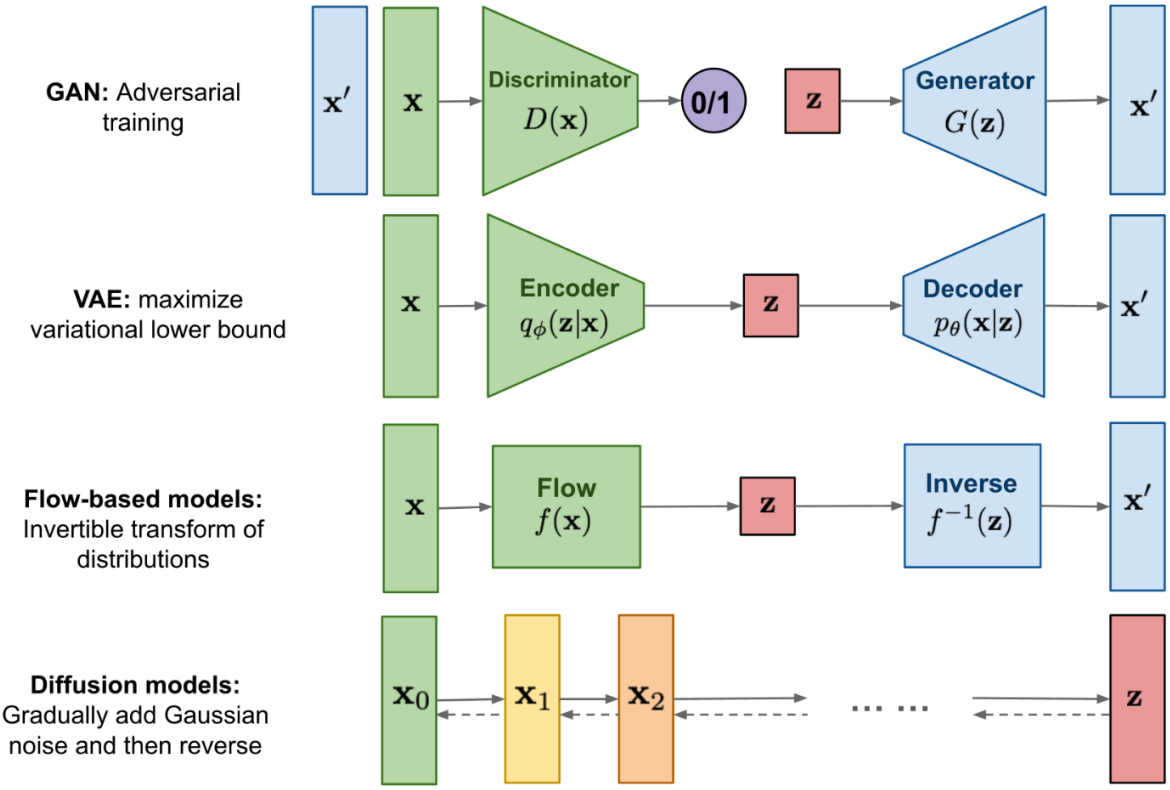
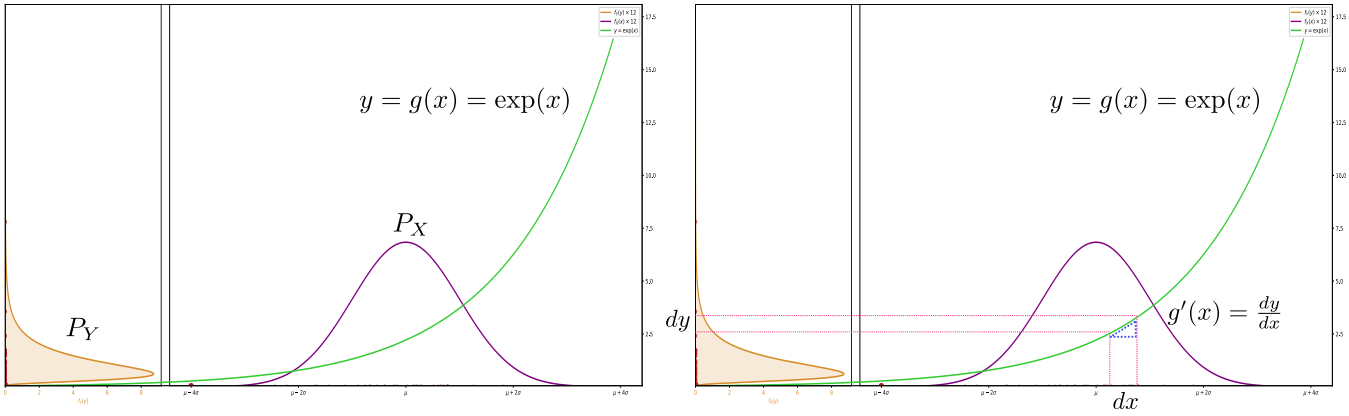


Figure 27.1: An overview of generative models.

- Flow-models get an exact estimate of the likelihood of your sample, as well as in the reverse direction.
- VAEs optimize a lower bound on the (log) likelihood
- GANs minimize a discrepancy between your input and transformed noise distributions.



27.1 The Method of Transformations of Random Variables

If we are interested in finding the PDF of $Y = g(X)$, where $g(\cdot)$ is some deterministic transformation of X, and the function g satisfies following properties, we can utilize a method called the method of transformations.

- $g(x)$ is differentiable;
- $g(x)$ is a strictly (or monotonically) increasing function, that is, if $x_1 < x_2$, then $g(x_1) < g(x_2)$.

How to derive the PDF of the random variable $Y = g(X)$ when one knows the PDF of the random variable X? If X is discrete, we can derive the pmf for Y by simply summing up the probability mass for all the x's such that $f(x) = y$. For a general function g, there is no direct formula to get the PDF of the random variable $Y = g(X)$ knowing $p(X)$. There is a formula in case when h is a differentiable one-to-one mapping from the range (*i.e.,* the support) of X to the range of Y.

Take for example a random variable $X \sim \mathcal{N}(\mu, \sigma)$ and set $Y = \exp(X)$. The figure below shows some simulations of X and the corresponding values of Y. The density of X is shown in blue and the one of Y is shown in orange in the vertical direction.

Now the question is: knowing the density of X, what is the density of Y? Taking a point y in the range of Y, the PDF f_Y provides the probability of Y, belong to a small area dy around y by the formula below

$$P(Y \in dy) \approx f_Y(y)|dy|,$$

where $P(Y \in dy)$ is the area below the curve. Similarly, we can define

$$P(X \in dx) \approx f_X(x)|dx|$$

The above two areas are approximately the same in case of very small region. Note that if dy and dx are very small, we can approximate the derivative of $g'(x) = \frac{|dy|}{|dx|}$. Compactly, this can be expressed as follows:

$$P(X \in dx) = f_X(x)\frac{|dy|}{g'(x)}$$

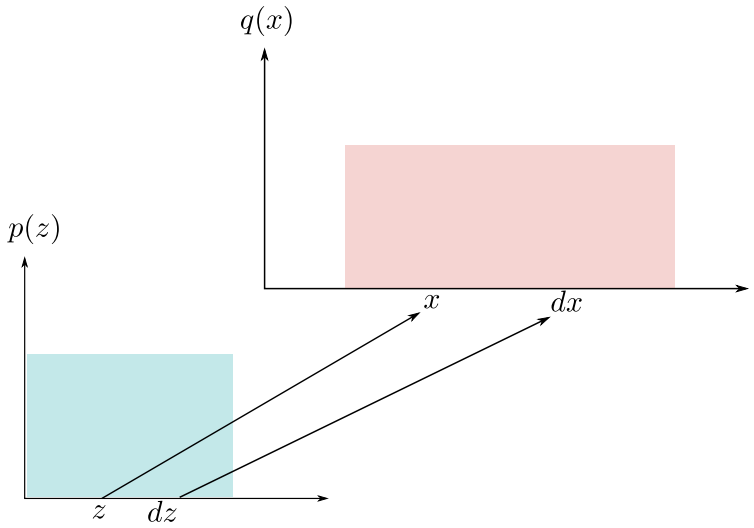


Figure 27.2: Area would be approximately $p(z)dz = q(z)dx$. Thus, $q(x) = p(z)\left|\frac{dz}{dx}\right|$

With $y = g(x)$ we can get

$$\begin{aligned} P(X \in dx) \approx P(Y \in dy) &= f_X(x)\frac{|dy|}{g'(x)} \\ &= f_X(g^{-1}(y))\frac{|dy|}{g'(g^{-1}(y))} \\ &= f_X(g^{-1}(y))|dy|(g^{-1})'(y) \end{aligned}$$

The last line is by the derivative of inverse function which is

$$\frac{d}{dx}f^{-1}(x) = \frac{1}{f'(f^{-1}(x))}$$

Then,

$$P(Y \in dy) \approx f_Y(y)|dy| = f_X(g^{-1}(y))|(g^{-1})'(y)| \cdot |dy|$$

Finally, we can get

$$f_Y(y) = f_X(g^{-1}(y))|(g^{-1})'(y)|$$

Note that the absolute is determined by the function h. It is a scaling factor tells us how a tiny volume element (like a little square or cube) is stretched or compressed under the transformation.

27.1.1 Vector to Vector

Z and X be random variables which are related by a mapping $f : \mathbb{R}^n \to \mathbb{R}^n$ such that $X = f(Z)$ and $Z = f^{-1}(X)$. Then

$$p_X(\mathbf{x}) = p_Z(f^{-1}(\mathbf{x}))\left|\det\left(\frac{\partial f^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

Note that for any invertible square matrix A over a field (*e.g.,* real or complex numbers),

$$\det\left(A^{-1}\right) = \frac{1}{\det(A)}.$$

Let

$$A = \begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix}.$$

Then, determinant of A is given by

$$\det(A) = 2 \cdot 4 - 3 \cdot 1 = 8 - 3 = 5.$$

The inverse of A is

$$A^{-1} = \frac{1}{5} \begin{bmatrix} 4 & -1 \\ -3 & 2 \end{bmatrix}.$$

Then, the determinant of A^{-1} is

$$\det(A^{-1}) = \frac{1}{5^2}\big(4 \cdot 2 - (-3)(-1)\big) = \frac{1}{25}(8 - 3) = \frac{5}{25} = \frac{1}{5}.$$

You can confirm the property:

$$\det(A^{-1}) = \frac{1}{5} = \frac{1}{\det(A)}.$$

For example, we can transform (x_1, x_2) to (r, θ) via $x_1 = r\cos\theta$ and $x_2 = r\sin\theta$.

Then

$$J_{y\to x} = \begin{pmatrix} \dfrac{\partial x_1}{\partial r} & \dfrac{\partial x_1}{\partial \theta} \\ \dfrac{\partial x_2}{\partial r} & \dfrac{\partial x_2}{\partial \theta} \end{pmatrix} = \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix}, \tag{3}$$

so

$$\big|\det J_{y\to x}\big| = \big|\, r\cos^2\theta + r\sin^2\theta \,\big| = |r|. \tag{4}$$

Hence

$$p_{\mathbf{y}}(\mathbf{y}) = p_{\mathbf{x}}(\mathbf{x})\,|J_{y\to x}| \quad \Longrightarrow \quad p_{R,\Theta}(r,\theta) = p_{X_1,X_2}(x_1,x_2)\, r. \tag{5–6}$$

For a two dimensional random vector (X, Y) with density $p_{X,Y}$,

$$Pr((X,Y) \in A) = \int\int_A p_{X,Y}(x,y)dxdy.$$

For a infinitesimally small region, we can approximate as follows:

$$\int_x^{x+dx} p_X(x)dx \approx p_X(x)dx.$$

Similarly, we can get the probability as follows:

$$P\big(r \le R \le r + dr,\ \theta \le \Theta \le \theta + d\theta\big) = p_{R,\Theta}(r,\theta)\, dr\, d\theta. \tag{7}$$

Note that the length of arc is $r \times d\theta$. Thus, the area $r\, dr\, d\theta$ or probability is given by

$$P\big(r \le R \le r + dr,\ \theta \le \Theta \le \theta + d\theta\big) = p_{X,Y}(r\cos\theta, r\sin\theta)\, r\, dr\, d\theta, \tag{8–9}$$

so that finally

$$p_{R,\Theta}(r,\theta) = p_{X,Y}(r\cos\theta, r\sin\theta)\, r. \tag{10}$$

27.2 Normalizing Flows

For a **univariate** case,

- Z: source random variable and density $p(z)$
- X: target random variable and density $q(x)$

$$T : Z \to X$$

- $$q(x) = p(z)\left|\frac{\partial T(z)}{\partial z}\right|^{-1}$$

For a **multivariate** case

$$\mathbf{T} : \mathbb{R}^d \to \mathbb{R}^d$$

So,

$$q(\mathbf{x}) = p(\mathbf{x})|\det \nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z})|^{-1}$$

For example,

- $\mathbf{X} \in \mathbb{R}^d$ and $\mathbf{Z} \in \mathbb{R}^d$
- $\mathbf{X} = (\mathbf{x}_1, ..., \mathbf{x}_d)$ and $\mathbf{Z} = (\mathbf{z}_1, ..., \mathbf{z}_d)$
- $\mathbf{T} = (T_1, T_2, ..., T_d)$
- $\mathbf{x}_1 = T_1(\mathbf{z})$, $\mathbf{x}_2 = T_2(\mathbf{z})$, $\mathbf{x}_d = T_d(\mathbf{z})$

Jacobian matrix of $\mathbf{T}$ is given by

$$\nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z}) = \begin{bmatrix} \frac{\partial T_1}{\partial z_1} & \frac{\partial T_1}{\partial z_2} & \cdots & \frac{\partial T_1}{\partial z_d} \\ \frac{\partial T_2}{\partial z_1} & \frac{\partial T_2}{\partial z_2} & \cdots & \frac{\partial T_2}{\partial z_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial T_d}{\partial z_1} & \frac{\partial T_d}{\partial z_2} & \cdots & \frac{\partial T_d}{\partial z_d} \end{bmatrix}$$

Our goal is to estimate the dataset $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_n\} \sim q(\mathbf{x})$

- Choose a simple density $p(z)$
- We want to estimate $q(\mathbf{x})$ by using MLE:

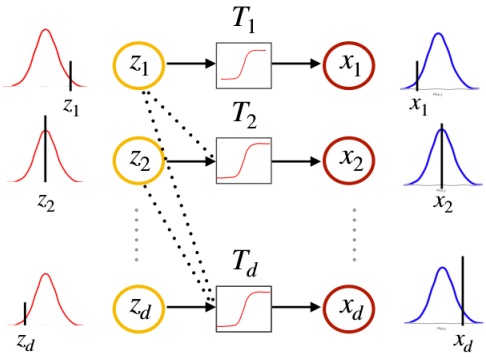
$$\prod_{i=1}^{n} q(\mathbf{x}_i) = \prod_{i=1}^{n} p(\mathbf{z}_i)|\det \nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z})|^{-1} \quad \text{by change of variable}$$

$$\hat{\mathbf{T}} := \underset{\mathbf{T}}{\operatorname{argmax}} \prod_{i=1}^{n} p(\mathbf{z}_i)|\det \nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z})|^{-1}$$

$$\hat{\mathbf{T}} := \underset{\mathbf{T}}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(\mathbf{z}_i) - \log|\det \nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z})|$$

- $\mathbf{z}_i = \mathbf{T}^{-1}(\mathbf{x}_i)$
- We need to compute the inverse $\mathbf{T}^{-1}$, which is computationally expensive
- We want to avoid the issue by using Jacobian trainagular matrix

$$q(x) = q_1(x_1) \cdot q_2(x_2 \mid x_1) \cdot \ldots \cdot q_d(x_d \mid x_{<d})$$



$$x_1 = \sigma_1 \cdot z_1 + \mu_1 =: T_1(z_1)$$

$$x_2 = \sigma_2(z_1) \cdot z_2 + \mu_2(z_1) := T_2(z_2 \,; z_1)$$

$$x_d = \sigma_d(z_{<d}) \cdot z_d + \mu_d(z_{<d}) := T_d(z_d \,; z_{<d})$$

27.2.1 Triangular Maps

$$\mathbf{T} : \mathbb{R}^d \to \mathbb{R}^d$$

$$\nabla_{\mathbf{z}} \mathbf{T}(\mathbf{z}) = \begin{bmatrix} \frac{\partial T_1}{\partial z_1} & 0 & \cdots & 0 \\ \frac{\partial T_2}{\partial z_1} & \frac{\partial T_2}{\partial z_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial T_d}{\partial z_1} & \frac{\partial T_d}{\partial z_2} & \cdots & \frac{\partial T_d}{\partial z_d} \end{bmatrix}$$

Increasing: T_j is w.r.t z_j. Determinant is the product of diagonal elements.

- $x_1 = T_1(z_1)$
- $x_2 = T_2(z_1, z_2)$
- $x_3 = T_2(z_1, z_2, z_3)$
- $x_d = T_2(z_1, z_2, ..., z_d)$

$$\min_{\mathbf{T}} \sum_{i=1}^{n} \left[-\log p(\mathbf{T}^{-1}(\mathbf{x}_i)) + \sum_j \log \frac{\partial T_j}{\partial z_j} \right]$$

Part V

Natural Language Processing

Chapter 28

Introduction

28.1 Evaluation Metrics

In the context of a bigram model, likelihood refers to the probability of observing a sequence of words in a corpus based on the bigram model's parameters. The bigram model assumes that the probability of a word in a sequence depends only on the immediately preceding word, making it a **Markov model of order 1**.

A bigram model represents the probability of a word sequence $W = (w_1, w_2, \ldots, w_n)$ as a product of conditional probabilities:

$$P(W) = P(w_1) \prod_{i=2}^{n} P(w_i|w_{i-1})$$

Here, $P(w_i|w_{i-1})$ is the conditional probability of word w_i given the preceding word w_{i-1}.

The **likelihood** of a sequence of words (data) $W = (w_1, w_2, \ldots, w_n)$ under the bigram model is:

$$L(\theta|W) = P(W|\theta) = P(w_1|\theta) \prod_{i=2}^{n} P(w_i|w_{i-1}, \theta)$$

Here, θ represents the model parameters, specifically the probabilities $P(w_i|w_{i-1})$.

Maximum Likelihood Estimation (MLE) in the Bigram Model To find the parameters $P(w_i|w_{i-1})$ that maximize the likelihood of the observed data, the **maximum likelihood estimation (MLE)** approach is commonly used.

The bigram probabilities $P(w_i|w_{i-1})$ are estimated from the frequency counts in the training corpus:

$$P(w_i|w_{i-1}) = \frac{\text{Count}(w_{i-1}, w_i)}{\text{Count}(w_{i-1})}$$

where:

- $\text{Count}(w_{i-1}, w_i)$ is the number of times the bigram (w_{i-1}, w_i) appears in the corpus.
- $\text{Count}(w_{i-1})$ is the number of times the word w_{i-1} appears.

To simplify computations, the log-likelihood of the sequence is used:

$$\log L(\theta|W) = \log P(w_1|\theta) + \sum_{i=2}^{n} \log P(w_i|w_{i-1}, \theta)$$

- Recall: TP/(TP+FN). Find all relevant cases whithin a dataset.
- Precision: TP/(TP+FP): While recall expresses the ability to find all relevant instances in a dataset, precision expresses the proportion of the data points our model says was relevant actually were relevant.
- The F1 score is the harmonic mean of precision and recall taking both metrics into account in the following equation:

28.1.1 Perplexity

Intuitively, perplexity can be understood as a *measure of uncertainty*. The perplexity of a language model can be seen as the level of perplexity. Consider a language model with an entropy of three bits, in which each bit encodes two possible outcomes of equal probability. This means that when predicting a symbol, that language model has to choose among $2^3 = 8$ possible options. Thus, we can argue that this language model has a perplexity of 8.

It can be modeled as $2^H(P, Q)$:

$$\begin{aligned} PPL(W) &= P(w_1, \cdots, w_N)^{-\frac{1}{N}} \\ &\approx \left(\prod_{i=1}^{N} P(w_i|w_{<i}) \right)^{-\frac{1}{N}} \\ &= \sqrt[n]{\frac{1}{\prod_{i=1}^{N} P(w_i|w_{<i})}} \end{aligned}$$

Let's derive it from a cross-entropy. We want to optimize P_θ instead of the true distribution P:

$$\begin{aligned} \mathcal{L}_{CE} &= -\mathbb{E}_{w\sim P}[P_\theta(w_i|w_{<i})] && (28.1) \\ &\approx -\frac{1}{N} \sum_{i=1}^{N} \log P_\theta(w_i|w_{<i}) && (28.2) \\ &= -\frac{1}{N} \log \prod_{i=1}^{N} P_\theta(w_i|w_{<i}) && (28.3) \\ &= \log \left(\prod_{i=1}^{N} P_\theta(w_i|w_{<i}) \right)^{-\frac{1}{N}} && (28.4) \\ &= \log \sqrt[N]{\frac{1}{\prod_{i=1}^{N} P_\theta(w_i|w_{<i})}} && (28.5) \\ & && (28.6) \end{aligned}$$

Thus, $PPL(W) = \exp\Big(\mathcal{L}_{CE}\Big)$.

28.1.2 Cross-Entropy and Perplexity

$$
\begin{aligned}
H(P,Q) &= -\sum_x P(x)\log Q(x) \\
&= -\sum_x P(x)[\log P(x) + \log Q(x) - \log P(x)] \\
&= -\sum_x P(x)\left[\log P(x) + \log \frac{Q(x)}{P(x)}\right] \\
&= H(P) + D_{KL}(P||Q)
\end{aligned}
$$

It should be noted that since the empirical entropy $H(P)$ is unoptimizable, when we train a language model with the objective of minimizing the cross entropy loss, the true objective is to minimize the KL-divergence of the distribution, which was learned by our language model from the empirical distribution of the language.

Chapter 29

Classical NLP Techniques

29.1 Edit Distance

Edit distance is a method used in spell correction to determine how similar two words are by calculating the minimum number of operations (insertions, deletions, or substitutions) required to transform one word into another. The smaller the edit distance, the more similar the two words are.

For example, let's say we have the following dictionary of valid words: "cat", "car", "cart", "care", "cards", "cast". If the input word is "carr", we calculate the edit distance between "carr" and each word in the dictionary as follows:

- cat: 3 (insert "r" and "r", then delete "t")
- car: 1 (replace second "r" with "t")
- cart: 2 (insert "t" and delete second "r")

The smallest edit distance is 1, between "carr" and "car", so "car" would be selected as the corrected word.

The edit distance method can be improved by using techniques such as weighting the importance of each operation (insertion, deletion, substitution) or using a more sophisticated algorithm such as *Levenshtein distance*. Additionally, the method can be combined with other methods such as language modeling or phonetic analysis to further improve spell correction accuracy.

29.2 Point-wise Mutual Information

Point-wise Mutual Information (PMI) is a statistical measure to calculate the association between two words in a given corpus. PMI is calculated by comparing the probability of the co-occurrence of two words with their individual probabilities of occurrence.

Formally, it is a quantity which is closely related to the mutual information is the point-wise

mutual information. For two events (not random variables) x and y, this is defined as

$$\text{PMI}[x, y] \triangleq \log \frac{p(x, y)}{p(x)p(y)} \tag{29.1}$$

$$= \frac{p(x|y)}{p(x)} = \frac{p(y|x)}{p(y)} \tag{29.2}$$

This measures the discrepancy between these events occurring together compared to what would be expected by chance.

- x and y are two words being considered,
- $P(x)$ is the probability of the occurrence of word x in the corpus,
- $P(y)$ is the probability of the occurrence of word y in the corpus, and
- $P(x, y)$ is the probability of the co-occurrence of words x and y in the corpus. In other words, x and y are adjacent

For terms with three words, the formula becomes:

$$\text{PMI}[x, y, z] = \log \frac{p(x, y, z)}{p(x)p(y)p(z)}$$

PMI values can range from $-\infty$ to ∞. Positive PMI values indicate that the words have a strong association, while negative values indicate that the words are unlikely to appear together.

For example, consider a small corpus of text:

- "The cat sat on the mat. The dog sat on the mat."
- The matrix below is 6×6 considering all possible combination of the "forward" co-occurrences.

$$\begin{bmatrix} & the & cat & dog & sat & on & mat \\ the & 0 & 1 & 1 & 0 & 0 & 2 \\ cat & 0 & 0 & 0 & 1 & 0 & 0 \\ dog & 0 & 0 & 0 & 1 & 0 & 0 \\ sat & 0 & 0 & 0 & 0 & 2 & 0 \\ on & 2 & 0 & 0 & 0 & 0 & 0 \\ mat & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

29.2.1 Remove Stopwords prior to PMI

In the above example we have not removed stopwords, so some of you might be wondering if we need to remove stopwords prior to PMI. It depends on the problem statement but if your objective is to find the related words, you should remove stopwords prior to calculating PMI.

29.3 TF-IDF

The term TF stands for term frequency, and the term IDF stands for inverse document frequency.

The TF-IDF representation takes into account the importance of each word in a document. In the bag-of-words model, each word is assumed to be equally important, which is obviously a less accurate assumption.

The method to calculate the TF-IDF weights of a term in a document is given by the following formula:

- **Term Frequency** (TF), $tf(t,d)$, is the relative frequency of term t within document d,

$$tf(t,d) = \frac{f_{t,d}}{\sum_{t' \in d} f_{t',d}},$$

  where $f_{t,d}$ is the raw count of a term in a document, *i.e.*,, the number of times that term t occurs in document d. Note the denominator is simply the total number of terms in document d (counting each occurrence of the same term separately). There are various other ways to define term frequency:

  - The raw count itself: $tf(t,d) = f_{t,d}$
  - Boolean "frequencies":

$$tf(t,d) = \begin{cases} 1, & \text{if } t \text{ occurs in } d \\ 0 & \text{otherwise} \end{cases}$$

  - Logarithmically scaled frequency: $tf(t,d) = \log(1 + ft, d)$
  - Augmented frequency, to prevent a bias towards longer documents, *e.g.*,. raw frequency divided by the raw frequency of the most frequently occurring term in the document:

$$tf(t,d) = 0.5 + 0.5\frac{f_{t,d}}{\max\{f_{t',d} : t' \in d\}}$$

- **Inverse document frequency (IDF)**: *The IDF is a measure of how much information the word provides*, *i.e.*,, if it is common or rare across all documents. It is the logarithmically scaled inverse fraction of the documents that contain the word, which is obtained by dividing the total number of documents by the number of documents containing the term, and then taking the logarithm of that quotient:

$$idf(t,D) = \log \frac{N}{|\{d \in D : t \in d\}|}$$

  - N total number of documents in the corpus ($= |D|$).
  - $|\{d \in D : t \in d\}|$: number of documents where the term t appears. If the term is not in the corpus, this will lead to a division-by-zero. It is therefore common to adjust the numerator $1 + N$ and denominator to $1 + |\{d \in D : t \in d\}|$.
  - Similarly, IDF can also be expressed

$$idf(t,D) = \log \frac{N - n + 0.5}{n + 0.5} + 1,$$

    where n is the number of documents containing the term t.

29.3.1 Term frequency–inverse document frequency

TF-IDF is calculated as a multiplication of $tf(t, D)$ and $idf(t, D)$.

- A high weight in TF–IDF is reached by a high term frequency (in the given document) and a low document frequency of the term in the whole collection of documents; the weights hence tend to filter out common terms.
- Since the ratio inside the IDF's log function is always greater than or equal to 1, the value of IDF (and TF–IDF) is greater than or equal to 0.
- As a term appears in more documents, the ratio inside the logarithm approaches 1, bringing the IDF and TF–IDF closer to 0.

In short, TF

- This measures the frequency of a word in a document. If a word appears more times in a document, it is likely more important to the document.
- number of times term "word" appears in a document / Total number of terms in the document
- Consider a document containing 100 words wherein the word 'cat' appears 3 times, then TF is 0.03

IDF:

- This measures the importance of a word in the entire corpus. If a word appears in many documents, it is likely less important to any individual document.
- $\log_e$ total number of documents/ Number of documents with term "word" in it.
- If we have 10 million documents, and 'cat' appears in 1,000 of these. Then, IDF is $\log 10,000,000/1,000 = 4$

Finally, TF-IDF is $0.03 \times 4 = 0.12$ The higher the TF-IDF score, the rarer the term and vice versa.

29.3.2 Link with Information Theory

This expression shows that summing the TF–IDF of all possible terms and documents recovers the mutual information between documents and term taking into account all the specificities of their joint distribution. Each TF–IDF hence carries the "bit of information" attached to a term x document pair.

29.4 Best Match 25 Ranking Algorithm

Best Match 25 ranking algorithm or BM25 is a bag-of-words retrieval function that ranks a set of documents based on the query terms appearing in each document, regardless of their proximity

within the document. It is a family of scoring functions with slightly different components and parameters. One of the most prominent instantiations of the function is as follows.

Given a query Q, containing keywords $q_1, \ldots, q_n$, the BM25 score of a document D is given by

$$\text{score}(D, Q) = \sum_{i=1}^{n} IDF(q_i) \cdot \frac{f(q_i, D) \cdot (k_1 + 1)}{f(q_i, D) + k_1 \cdot (1 - b + b \cdot \frac{|D|}{avgd1})},$$

where $f(q_i, D)$ is the number of times that the keyword q_i occurs in the document, D, $|D|$ is the length of the document D in words, and $avgd1$ is the average document length in a collection of documents. k_1 and b are free parameters, usually chosen, in absence of an advanced optimization, as $k_1 \in [1.2, 2.0]$ and $b = 0.75$.

29.5 Reciprocal Rank Fusion

Reciprocal Rank Fusion (RRF), a simple method for combining the document rankings from multiple information retrieval systems.

$$RRF(d \in D) = \sum_{r \in R} \frac{1}{k + r(d)}$$

- k is a constant that helps to balance between high and low ranking. Typically set at 60.
- $r(d)$ is the rank/position of the document.

29.6 PageRank and TextRank

29.7 Label Smoothing

For each training example x, our model computes the probability of each label $k \in \{1, ..., K\}$, $p(k|x) = \frac{\exp(z_k)}{\sum_i \exp(z_i)}$. Here z_k are the logits.

Label smoothing is a mechanism to regularize the classifier layer by estimating the marginalized effect of label-dropout during training.

Vanila corss-entropy can cause two problem:

- First, it may result in over-fitting: if the model learns to assign full probability to the ground-truth label for each training example, it is not guaranteed to generalize.
- Second, it encourages the differences between the largest logit and all others to become large, and this, combined with the bounded gradient $\frac{\partial \ell}{\partial z_k}$, reduces the ability of the model to adapt. Intuitively, this happens because the model becomes too confident about its predictions.

We propose a mechanism for encouraging the model to be less confident. While this may not be desired if the goal is to maximize the log-likelihood of training labels, it does regularize the model and makes it more adaptable. The method is very simple. Consider a distribution over labels $u(k)$, independent of the training example x, and a smoothing parameter ϵ. For a training example with ground-truth label y, we replace the label distribution $q(k|x) = \delta_{k,y}$ with

$$q'(k|x) = (1 - \epsilon)\delta_{k,y} + \epsilon u(k)$$

which is a mixture of the original ground-truth distribution $q(k|x)$ and the fixed distribution $u(k)$, with weights $1 - \epsilon$ and ϵ, respectively. This can be seen as the distribution of the label k obtained as follows:

$$q'(k|x) = (1 - \epsilon)\delta_{k,y} + \frac{\epsilon}{K}$$

We refer to this change in ground-truth label distribution as label-smoothing regularization, or LSR.

29.7.1 Another Interpretation

Instead of using one-hot encoded vector, we introduce noise distribution $u(y|x)$. Our new ground truth label for data (x_i, y_i) would be

$$\begin{aligned} p'(y|x_i) &= (1 - \varepsilon)p(y|x_i) + \varepsilon u(y|x_i) \\ &= \begin{cases} 1 - \varepsilon + \varepsilon u(y|x_i) & \text{if } y = y_i \\ \varepsilon u(y|x_i) & \text{otherwise} \end{cases} \end{aligned}$$

Where ε is a weight factor, $\varepsilon \in [0, 1]$, and note that $\sum_{y=1}^{K} p'(y|x_i) = 1$.

Chapter 30

POS Tagging

30.1 Introduction

Part-of-speech (POS) tagging is the process of labeling words in a text with their corresponding parts of speech in natural language processing (NLP). It helps algorithms understand the grammatical structure and meaning of a text.

Chapter 31

Language Model

31.1 Language Model

31.2 Tokenizers

31.3 Byte Pair Encoding

31.4 Byte Pair Encoding

Chapter 32

Transformer

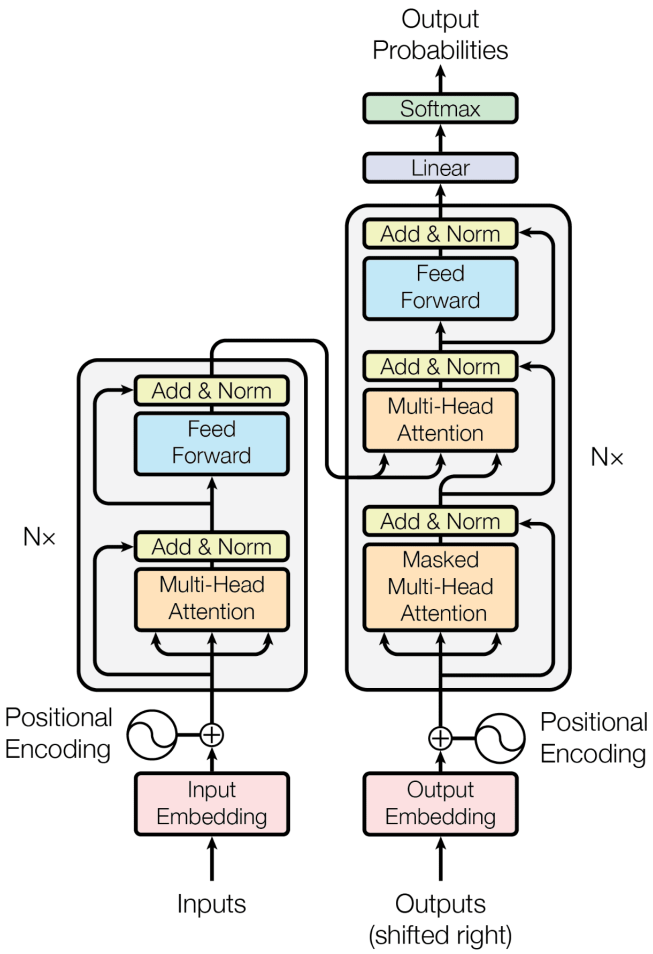


Figure 32.1: An illustration of Transformer architecture.

TLDR

- *Attention is a communication mechanism*, which can be seen as nodes in a directed graph looking at each other and aggregating information with a weighted sum from all nodes that point to them, with data-dependent weights.
- There is no notion of space. Attention simply acts over a set of vectors. This is why we need to positionally encode tokens.
- Each example across batch dimension is of course processed completely independently and never "talk" to each other
- In an "encoder" attention block just delete the single line that does masking with 'tril', allowing all tokens to communicate. This block here is called a "decoder" attention block because it has triangular masking, and is usually used in autoregressive settings, like language modeling.
- "self-attention" just means that the keys and values are produced from the same source as queries. In "cross-attention", the queries still get produced from x, but the keys and values come from some other, external source (*e.g.,* an encoder module)
- "Scaled" attention additional divides 'wei' by $1/sqrt(head\_size)$. This makes it so when

input Q,K are unit variance, wei will be unit variance too and Softmax will stay diffuse and not saturate too much. Illustration below

32.1 Attention Mechanism

The attention mechanism assigns *attention scores* (*i.e., weights*) to different parts of the input sequence, indicating how much each part contributes to the current output. In essence, the model "pays attention" to certain parts of the input more than others while processing each token in the sequence.

Assume the encoder produces 3 hidden states (each a 2-dimensional vector):

$$h_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad h_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad h_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Let the decoder's previous hidden state at time $t-1$ be:

$$s_{t-1} = \begin{bmatrix} 0.5 \\ 0.2 \end{bmatrix}.$$

Using the *dot product* as our score function, the alignment score for each encoder hidden state is:

$$e_{tj} = s_{t-1}^{\top} h_j.$$

Compute each:

1. For h_1:
$$e_{t1} = [0.5 \quad 0.2] \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0.5.$$
2. For h_2:
$$e_{t2} = [0.5 \quad 0.2] \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0.2.$$
3. For h_3:
$$e_{t3} = [0.5 \quad 0.2] \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0.7.$$

The attention weight for each encoder time step is given by:

$$\alpha_{tj} = \frac{\exp(e_{tj})}{\sum_{k=1}^{3} \exp(e_{tk})}.$$

Calculate the exponentials:

- $\exp(0.5) \approx 1.6487$,
- $\exp(0.2) \approx 1.2214$,

- $\exp(0.7) \approx 2.0138$.

Sum of exponentials:

$$S = 1.6487 + 1.2214 + 2.0138 \approx 4.8839.$$

Now compute each attention weight:

1. For α_{t1}:
$$\alpha_{t1} = \frac{1.6487}{4.8839} \approx 0.3374.$$
2. For α_{t2}:
$$\alpha_{t2} = \frac{1.2214}{4.8839} \approx 0.2501.$$
3. For α_{t3}:
$$\alpha_{t3} = \frac{2.0138}{4.8839} \approx 0.4125.$$

These weights sum to 1 (up to rounding):

$$0.3374 + 0.2501 + 0.4125 \approx 1.0000.$$

The context vector c_t is the weighted sum of the encoder hidden states:

$$c_t = \alpha_{t1} h_1 + \alpha_{t2} h_2 + \alpha_{t3} h_3.$$

Substitute in the values:

$$\begin{aligned} c_t &= 0.3374 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 0.2501 \begin{bmatrix} 0 \\ 1 \end{bmatrix} + 0.4125 \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 0.3374 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0.2501 \end{bmatrix} + \begin{bmatrix} 0.4125 \\ 0.4125 \end{bmatrix} \\ &= \begin{bmatrix} 0.3374 + 0.4125 \\ 0 + 0.2501 + 0.4125 \end{bmatrix} \\ &= \begin{bmatrix} 0.7499 \\ 0.6626 \end{bmatrix}. \end{aligned}$$

So, the context vector is approximately:

$$c_t \approx \begin{bmatrix} 0.75 \\ 0.66 \end{bmatrix}.$$

In a typical decoder, the context vector c_t is combined with the previous hidden state and possibly the previously generated output to update the current hidden state. For example, an update could be:

$$s_t = f(s_{t-1}, y_{t-1}, c_t),$$

or, if you are using a simple formulation with a combined input, it might be:

$$s_t = \tanh(W[s_{t-1}; c_t]),$$

where $[s_{t-1}; c_t]$ denotes the concatenation of s_{t-1} and c_t, and W is a learnable weight matrix. The updated state s_t would then be used to predict the next output token.

Let's use a machine translation task (English to French) as an example. Suppose we are translating the sentence "I am learning" into French.

- Input: Sequence of words in English: '[I, am, learning]'
- Output: Sequence of words in French: '[Je, suis, en, train, d'apprendre]'

Instead of compressing all the input information into a fixed-size context vector (like in traditional encoder-decoder models), the attention mechanism allows the decoder to look at different parts of the input sentence at each step of the decoding process.

	I	am	learning
Je	0.7	0.2	0.1
suis	0.1	0.8	0.1
en	0.05	0.15	0.8

This matrix shows that "Je" strongly attends to "I", "suis" attends mostly to "am", and "en" attends primarily to "learning".

32.1.1 Self-Attention

- n: the number of tokens in the sequence.
- d_{model}: the dimension of the input embeddings.
- d_k: the dimension of the query and key vectors.
- d_v: the dimension of the value vectors (often $d_k = d_v$, but they need not be equal).

Assume we have an input sequence of n tokens. For each token i (with $1 \leq i \leq n$) we start with an embedding vector $\mathbf{x}_i \in \mathbb{R}^{d_{\text{model}}}$. In self-attention, we first linearly project these embeddings into three different spaces to obtain the *query*, *key*, and *value* vectors:

$$\begin{aligned}
\mathbf{q}_i &= \mathbf{x}_i W^Q, \\
\mathbf{k}_i &= \mathbf{x}_i W^K, \\
\mathbf{v}_i &= \mathbf{x}_i W^V,
\end{aligned}$$

where

- $W^Q, W^K \in \mathbb{R}^{d_{\text{model}} \times d_k}$ are the query and key projection matrices,
- $W^V \in \mathbb{R}^{d_{\text{model}} \times d_v}$ is the value projection matrix,
- d_k (and sometimes d_v) is a chosen dimensionality for these spaces.

For a given token i, we compute its output representation as a weighted sum of the value vectors of all tokens. The weights are determined by the similarity between the query $\mathbf{q}_i$ and the keys $\mathbf{k}_j$ of all tokens j in the sequence.

First, compute the *dot-product scores* between the query for token i and every key:

$$s_{ij} = \mathbf{q}_i \cdot \mathbf{k}_j, \quad \text{for } j = 1, 2, \ldots, n.$$

To prevent the dot products from growing too large in magnitude (especially when d_k is large), we *scale the scores* by $\sqrt{d_k}$:

$$\tilde{s}_{ij} = \frac{s_{ij}}{\sqrt{d_k}}.$$

Next, we apply the softmax function over the scaled scores for token i to obtain the attention weights α_{ij}:

$$\alpha_{ij} = \frac{\exp(\tilde{s}_{ij})}{\sum_{l=1}^{n} \exp(\tilde{s}_{il})}.$$

These weights satisfy $\sum_{j=1}^{n} \alpha_{ij} = 1$.

Finally, the output for token i, denoted by $\mathbf{z}_i$, is the weighted sum of the value vectors:

$$\mathbf{z}_i = \sum_{j=1}^{n} \alpha_{ij} \, \mathbf{v}_j.$$

In matrix form for all tokens, if we define matrices Q, K, and V whose rows are the vectors $\mathbf{q}_i$, $\mathbf{k}_i$, and $\mathbf{v}_i$ respectively, the self-attention operation is:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V.$$

Here, $Q, K, V \in \mathbb{R}^{n \times d_{model}}$, QK^T's time complexity is $O(N^2 d)$. This quadratic cost is massive for long input-sequences such as documents to be summarized or character-level inputs.

Input Embeddings Each token i is represented by an embedding:

$$\mathbf{x}_i \in \mathbb{R}^{d_{\text{model}}}.$$

You can think of all the tokens put together as a matrix:

$$X \in \mathbb{R}^{n \times d_{\text{model}}}.$$

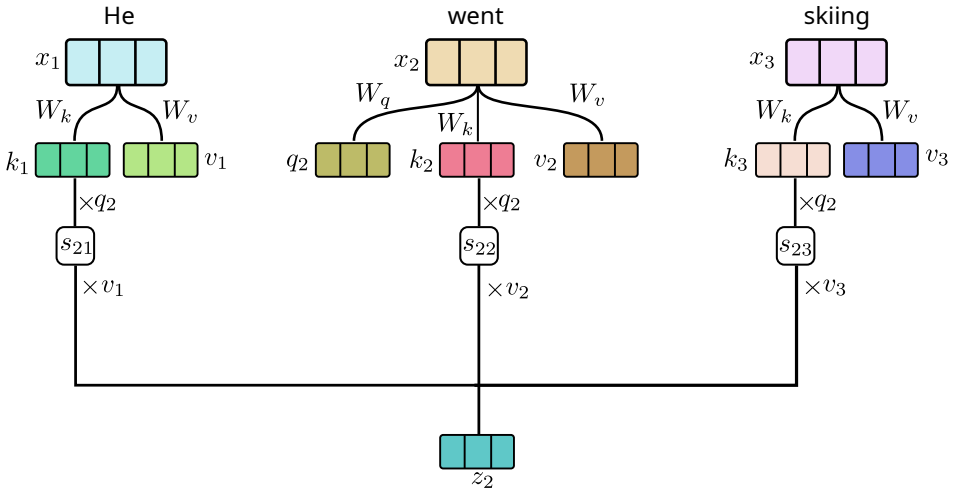


Figure 32.2: An Illustration of the self-attention.

Projection Matrices To obtain the queries, keys, and values, we use learned projection matrices:

$$W^Q \in \mathbb{R}^{d_{\text{model}} \times d_k},$$
$$W^K \in \mathbb{R}^{d_{\text{model}} \times d_k},$$
$$W^V \in \mathbb{R}^{d_{\text{model}} \times d_v}.$$

Projected Matrices Multiplying the input X by these weight matrices gives:

$$Q = X\,W^Q \in \mathbb{R}^{n \times d_k},$$
$$K = X\,W^K \in \mathbb{R}^{n \times d_k},$$
$$V = X\,W^V \in \mathbb{R}^{n \times d_v}.$$

Here, each row of Q (or K, or V) corresponds to the query (or key, or value) of one token.

Dot-Product Attention Scores The attention scores between tokens are computed using:

$$QK^\top \in \mathbb{R}^{n \times n}.$$

In this product:

- Q is $n \times d_k$
- $K^\top$ is $d_k \times n$

Therefore, the result is an $n \times n$ matrix where each entry (i, j) represents the (unnormalized) similarity between token i and token j.

Scaled Dot-Product and Softmax Before applying the softmax, the scores are scaled by $\sqrt{d_k}$:

$$\frac{QK^\top}{\sqrt{d_k}} \in \mathbb{R}^{n \times n}.$$

Then, applying the softmax function row-wise produces an attention weight matrix $A \in \mathbb{R}^{n \times n}$:

$$A = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right).$$

Final Output Finally, the output of the self-attention layer is computed as:

$$\text{Attention}(Q, K, V) = A\,V.$$

Since:

- A is $n \times n$,
- V is $n \times d_v$,

The final output is:

$$\text{Attention}(Q, K, V) \in \mathbb{R}^{n \times d_v}.$$

32.1.2 Masked Attention

In autoregressive tasks (*e.g.,* language modeling), it is essential that when predicting a token at position ii, the model does not "peek" at any tokens at positions $j > i$. *Masked attention* ensures that each token only attends to tokens at the same or earlier positions. The masked attention is often referred to *cross-attention*. This is just a self-attention in decoder.

$$\text{MA}(Q, K, V) = softmax\left(\frac{Q^T K + M}{\sqrt{d_k}}\right)V,$$

where M

$$M_{ij} = \begin{cases} 0 & \text{if } j \leq i \\ -\infty & \text{if } j > i \end{cases}$$

Note that $-\infty$ will make *exp* term to be zero.

32.1.3 Multi-Head Attention

Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions. **Rather than computing a single attention function with full-dimensional queries, keys, and values, the mechanism splits them into multiple "heads" and computes attention in parallel**.

Suppose:

- The input embeddings (or previous layer outputs) form the matrix $X \in \mathbb{R}^{n \times d_{\text{model}}}$,
- d_{model} is the model (or embedding) dimension,
- We decide to use h attention heads.

Each head will work with lower-dimensional projections of the input. In particular, we typically set:

$$d'_k = d'_v = \frac{d_{\text{model}}}{h},$$

so that each head processes queries, keys, and values of dimensions d'_k and d'_v, and the total computation remains efficient.

Linear Projections for Each Head For each head $i \in \{1, \ldots, h\}$, we define learned projection matrices:

$$W_i^Q \in \mathbb{R}^{d_{\text{model}} \times d'_k},$$
$$W_i^K \in \mathbb{R}^{d_{\text{model}} \times d'_k},$$
$$W_i^V \in \mathbb{R}^{d_{\text{model}} \times d'_v}.$$

We then project the input X to obtain:

$$Q_i = XW_i^Q \in \mathbb{R}^{n \times d'_k},$$
$$K_i = XW_i^K \in \mathbb{R}^{n \times d'_k},$$
$$V_i = XW_i^V \in \mathbb{R}^{n \times d'_v}.$$

Compute Scaled (Masked) Dot-Product Attention for Each Head For each head i, compute:

$$\text{head}_i = \text{Attention}(Q_i, K_i, V_i),$$

where the attention function is defined as:

$$\text{head}_i = \text{softmax}\left(\frac{Q_i K_i^\top + M}{\sqrt{d'_k}}\right) V_i.$$

- If masking is not required (*e.g.,* in the encoder or in *non-autoregressive* settings), simply set $M = 0$.
- *For decoder self-attention in autoregressive models*, M is defined as in the Masked Attention section above.

Concatenate the Heads and Project Once all heads are computed, we concatenate their outputs:

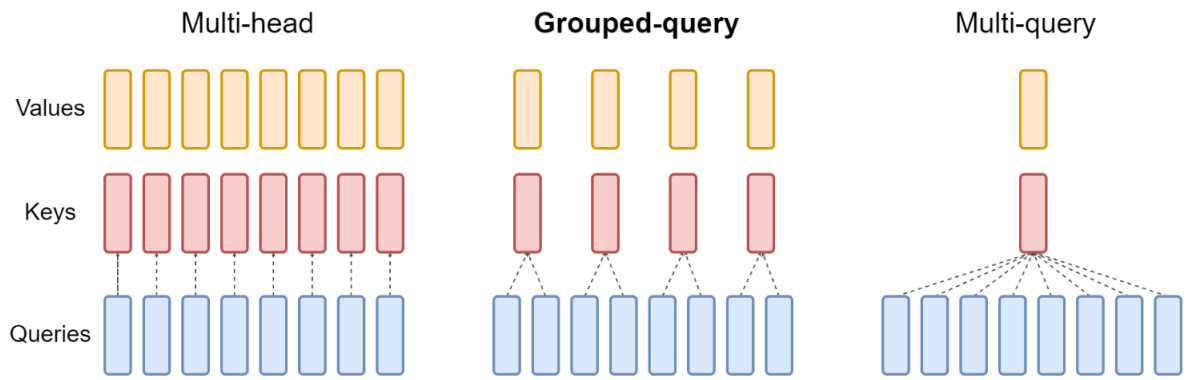
$$\text{Concat}(\text{head}_1, \text{head}_2, \ldots, \text{head}_h) \in \mathbb{R}^{n \times (h \cdot d'_v)}.$$

Finally, we apply a learned linear projection:

$$W^O \in \mathbb{R}^{(h \cdot d'_v) \times d_{\text{model}}},$$

to obtain the final multi-head attention output:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h) W^O \in \mathbb{R}^{n \times d_{\text{model}}}.$$



32.2 Various Attention Mechanisms

If we use a single value and a single key over all queries, we can significantly reduce the memory usage for KV caching. This is the basic idea of the multi-query attention (MQA) and the grouped query attention (GQA). However, MQA tends to lower the output quality as the model size increases. GQA achieved a balance between them.

32.3 Positional Embedding

The self-attention mechanism in transformers treats all tokens in a sequence in parallel without an inherent notion of order. This means that, by itself, self-attention is invariant to the order of input tokens. Positional encoding is introduced to inject order information so that the model can differentiate between tokens based on their positions.

- **Absolute Positional Embeddings**: Each position in the sequence is assigned a unique vector. Although straightforward, these embeddings don't scale well to longer sequences and fail to capture the nuances of relative positions between tokens.
- **Relative Positional Embeddings**: These embeddings focus on the distance between tokens, which can improve the model's understanding of token relationships. However, they typically introduce additional complexity into the model architecture.

32.3.1 Permutation Invariance of Self-Attention

Without positional embeddings, the transformer's self-attention would treat the input as a bag of tokens, ignoring the order entirely. The added positional embeddings break this permutation invariance by encoding the position directly into the token representation. As a result, even if the same tokens are present, the model can infer their relative order and roles in the sentence.

Imagine you have a short sentence, "I feel good". If you simply pass this sentence into a transformer, the model wouldn't know the order of the words. The same set of token (*i.e.,* word) embeddings could represent the sentence "good feel I" if no ordering information were provided.

We formulate this as follows: With a permutation matrix P of shape (n, n), the input tokens can be permuted as

$$X' = PX.$$

Let's follow the same self-attention process for X':

$$Q' = X'W_q = PXW_q = PQ,$$

$$K' = X'W_k = PXW_k = PK,$$

$$V' = X'W_v = PXW_v = PV.$$

Then, compute the scores using Q' and K':

$$S' = \frac{Q'(K')^T}{\sqrt{d_k}} = \frac{(PQ)(PK)^T}{\sqrt{d_k}}.$$

Note that

$$(PK)^T = K^T P^T,$$

so

$$S' = \frac{PQK^T P^T}{\sqrt{d_k}} = P\,S\,P^T.$$

The softmax is applied row-wise.

$$A' = \text{Softmax}(S').$$

Since P and P^T are just reordering rows and columns, respectively, the attention weights A are simply permuted like below:

$$A' = P\,A\,P^T.$$

Finally, the output for the permuted input is:

$$\text{Attention}(X') = A'V' = (PAP^T)(PV) = PAV = P\,\text{Attention}(X).$$

As you can see the self-attention mechanism is *equivariant* to permutations. This means that if you permute the input tokens, the output is permuted in the same way. There is no mechanism in the equations above that distinguishes one ordering from another; the operations treat all tokens symmetrically.

Thus, without additional positional encodings, if you were to shuffle the tokens, the model would compute the same set of pairwise interactions—just in a different order. The structure of the equations does not provide any mechanism for the model to know that one token came before or after another.

32.3.2 Sinusoidal Positional Encoding

In a Transformer model, positional encoding vectors are added to the token (word) embeddings before the input is fed into the self-attention layers. This addition gives the model a sense of the order in the sequence, enabling it to capture the sequential relationships between tokens despite processing them in parallel.

- $\text{PE}(pos, 2i) = \sin\left(\frac{pos}{10000^{\frac{2i}{d_{\text{model}}}}}\right)$
- $\text{PE}(pos, 2i+1) = \cos\left(\frac{pos}{10000^{\frac{2i}{d_{\text{model}}}}}\right)$,

where:

- pos: the position of the token in the sequence (starting at 0),
- i: the index along the embedding dimension,
- d_{model}: the total dimension of the model's embeddings.

Let's work through a concrete example with a very small embedding dimension:

- Assume $d_{\text{model}} = 4$.
- We'll compute the positional encoding for two positions: $pos = 0$ and $pos = 1$.

Since $d_{\text{model}} = 4$, we have 4 dimensions indexed $0, 1, 2, 3$. The formulas split the dimensions into even and odd indices:

For $pos = 0$

- Dimension 0 (even index, $i = 0$):

$$\text{PE}(0,0) = \sin\Big(\frac{0}{10000^{\frac{2\cdot 0}{4}}}\Big) = \sin\Big(\frac{0}{10000^{0}}\Big) = \sin(0) = 0.$$

- Dimension 1 (odd index, $i = 0$):

$$\text{PE}(0,1) = \cos\Big(\frac{0}{10000^{\frac{2\cdot 0}{4}}}\Big) = \cos(0) = 1.$$

- Dimension 2 (even index, $i = 1$):

$$\text{PE}(0,2) = \sin\Big(\frac{0}{10000^{\frac{2\cdot 1}{4}}}\Big) = \sin\Big(\frac{0}{10000^{0.5}}\Big) = \sin(0) = 0.$$

- Dimension 3 (odd index, $i = 1$):

$$\text{PE}(0,3) = \cos\Big(\frac{0}{10000^{\frac{2\cdot 1}{4}}}\Big) = \cos(0) = 1.$$

- So, the positional encoding for $pos = 0$ is:

$$[0,\ 1,\ 0,\ 1].$$

For $pos = 1$

- Dimension 0 (even index, $i = 0$):

$$\text{PE}(1,0) = \sin\Big(\frac{1}{10000^{\frac{2\cdot 0}{4}}}\Big) = \sin\Big(\frac{1}{10000^{0}}\Big) = \sin(1) \approx 0.84147.$$

- Dimension 1 (odd index, $i = 0$):

$$\text{PE}(1,1) = \cos\Big(\frac{1}{10000^{\frac{2\cdot 0}{4}}}\Big) = \cos(1) \approx 0.54030.$$

- Dimension 2 (even index, $i = 1$):

$$\text{PE}(1,2) = \sin\Big(\frac{1}{10000^{\frac{2\cdot 1}{4}}}\Big) = \sin\Big(\frac{1}{10000^{0.5}}\Big) = \sin\Big(\frac{1}{100}\Big) = \sin(0.01) \approx 0.00999983.$$

- Dimension 3 (odd index, $i = 1$):

$$\text{PE}(1,3) = \cos\Big(\frac{1}{10000^{\frac{2\cdot 1}{4}}}\Big) = \cos(0.01) \approx 0.99995.$$

- Thus, the positional encoding for $pos = 1$ is approximately:

$$[0.84147,\ 0.54030,\ 0.00999983,\ 0.99995].$$

32.3.3 RoPE

Rather than adding a positional vector to the token embeddings, **RoPE rotates the embeddings by a position-specific angle.** Think of it as "twisting" the embedding in space based on its position. For instance, if you have a simple two-dimensional embedding for the word "dog", you can imagine its vector being rotated by an angle θ if it's the first word, 2θ if it's the second word, and so on.

For high-dimensional embeddings (*e.g.,* in $\mathbb{R}^d$), RoPE divides the vector into $d/2$ pairs (or 2D subspaces). For a token at position i, denote its embedding by:

$$\mathbf{x}_i \in \mathbb{R}^d.$$

We partition $\mathbf{x}_i$ into pairs:

$$\mathbf{x}_i^{(k)} = \begin{pmatrix} x_{i,2k} \\ x_{i,2k+1} \end{pmatrix}, \quad k = 0, 1, \ldots, \frac{d}{2} - 1.$$

Subsequently, for each 2D subspace indexed by k, RoPE defines a rotation angle:

$$\theta_{i,k} = i \cdot \alpha_k,$$

where α_k is a scaling factor that typically depends on the dimension k. A popular choice is:

$$\alpha_k = \frac{1}{10000^{\frac{2k}{d}}}.$$

This scaling mimics the frequency scaling in sinusoidal embeddings (*i.e.,* positional embedding), ensuring that different subspaces capture positional information at different granularities.

In two-dimensional geometry, any rotation by an angle θ can be represented by a *rotation matrix* $R(\theta)$. This matrix is a standard tool in linear algebra and has the form:

$$R(\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}.$$

- Geometric Interpretation: The rotation matrix $R(\theta)$ rotates any 2D vector by the angle θ (in the counterclockwise direction) while preserving its magnitude. This property makes it ideal for encoding positional shifts—rotating a vector does not change its "content" (its norm) but changes its direction, thereby encoding positional information.
- Inherent Relative Encoding: When different positions correspond to different rotation angles, the relationship between any two positions can be captured by the difference in their rotation angles. This leads to a natural encoding of relative position without having to explicitly compute or store separate relative position vectors.

However, Transformer embeddings are typically high-dimensional. Thus, RoPE adopts a simple trick. They split the high dimensional vector into two halves so that each pair forms a 2D subspace. Thus, we can apply the rotation matrix.

For each 2D subspace, the rotary transformation is applied as follows. Given the subvector:

$$\mathbf{x}_i^{(k)} = \begin{pmatrix} x_{i,2k} \\ x_{i,2k+1} \end{pmatrix},$$

we compute its rotated version:

$$\mathrm{RoPE}_i\big(\mathbf{x}_i^{(k)}\big) = R(\theta_{i,k})\,\mathbf{x}_i^{(k)} = \begin{pmatrix}\cos(\theta_{i,k}) & -\sin(\theta_{i,k})\\ \sin(\theta_{i,k}) & \cos(\theta_{i,k})\end{pmatrix}\begin{pmatrix}x_{i,2k}\\ x_{i,2k+1}\end{pmatrix}.$$

This yields the updated coordinates:

$$\tilde{x}_{i,2k} = x_{i,2k}\cos(\theta_{i,k}) - x_{i,2k+1}\sin(\theta_{i,k}),$$

$$\tilde{x}_{i,2k+1} = x_{i,2k+1}\cos(\theta_{i,k}) + x_{i,2k}\sin(\theta_{i,k}).$$

After processing all $d/2$ subspaces, we concatenate the results back into a full d-dimensional vector $\tilde{\mathbf{x}}_i$.

In transformer architectures, RoPE is applied to both the query and the key vectors except the value vecotrs:

$$\tilde{\mathbf{q}}_i = \mathrm{RoPE}_i(\mathbf{q}_i),$$
$$\tilde{\mathbf{k}}_j = \mathrm{RoPE}_j(\mathbf{k}_j).$$

Then, the attention score between positions i and j is calculated as:

$$\mathrm{Attention}(i,j) = \frac{\tilde{\mathbf{q}}_i \cdot \tilde{\mathbf{k}}_j}{\sqrt{d}}.$$

A key property of RoPE is that the dot product between the rotated vectors can be reinterpreted to show how relative positions are encoded. In particular, one can derive that:

$$\tilde{\mathbf{q}}_i^\top \tilde{\mathbf{k}}_j = \mathbf{q}_i^\top\, \mathbf{M}(i,j)\,\mathbf{k}_j,$$

where $\mathbf{M}(i,j)$ is a block diagonal matrix that encapsulates the effect of the relative positional difference $j-i$.

Focus on one 2D subspace (indexed by k):

- The query subvector at position i is rotated by $\theta_{i,k} = i\alpha_k$.
- The key subvector at position j is rotated by $\theta_{j,k} = j\alpha_k$.

The dot product in this subspace is:

$$\tilde{\mathbf{q}}_i^{(k)\top}\tilde{\mathbf{k}}_j^{(k)} = \Big(\mathbf{q}_i^{(k)}\Big)^\top R(\theta_{i,k})^\top R(\theta_{j,k})\,\mathbf{k}_j^{(k)}.$$

Since the transpose of a rotation matrix is its inverse (i.e., $R(\theta)^\top = R(-\theta)$), we have:

$$R(\theta_{i,k})^\top R(\theta_{j,k}) = R(-\theta_{i,k})R(\theta_{j,k}) = R\big(\theta_{j,k} - \theta_{i,k}\big).$$

Because $\theta_{j,k} - \theta_{i,k} = (j-i)\alpha_k$, the transformation becomes:

$$R\big((j-i)\alpha_k\big).$$

Repeating this for each 2D subspace results in a block diagonal matrix:

$$\mathbf{M}(i,j) = \mathrm{diag}\Big(R\big((j-i)\alpha_0\big),\, R\big((j-i)\alpha_1\big),\, \ldots,\, R\big((j-i)\alpha_{\frac{d}{2}-1}\big)\Big).$$

Each block is the 2×2 rotation matrix:

$$R\big((j-i)\alpha_k\big) = \begin{pmatrix}\cos\big((j-i)\alpha_k\big) & -\sin\big((j-i)\alpha_k\big)\\ \sin\big((j-i)\alpha_k\big) & \cos\big((j-i)\alpha_k\big)\end{pmatrix}.$$

- Relative Positional Bias: The matrix $\mathbf{M}(i, j)$ adjusts the dot product between queries and keys based on their relative positions $(j - i)$. Thus, the value vectors are not modified. Instead of explicitly adding a relative position embedding, the rotation inherently modulates the interaction between tokens.
- Unified Encoding: Since $\mathbf{M}(i, j)$ is built from standard rotation matrices $R(\theta)$, it seamlessly encodes the relative positional difference across all 2D subspaces. This results in a unified treatment where both absolute and relative positional cues are embedded into the attention calculation.
- Elegant Mathematical Foundation: The use of $R(\theta)$ comes directly from classical geometry and linear algebra. It leverages the well-known properties of rotations in 2D—specifically, that rotations preserve vector norms and that the composition of rotations is itself a rotation (with the angle being the sum or difference of the individual angles). This mathematical elegance translates into an efficient and effective mechanism for positional encoding.

32.3.4 Encoder

32.3.5 Decoder

The output of each step is fed to the bottom decoder in the next time step, and the decoders bubble up their decoding results just like the encoders did. And just like we did with the encoder inputs, we embed and add positional encoding to those decoder inputs to indicate the position of each word.

```
def forward(self, tgt: Tensor, memory: Tensor) -> Tensor:
  seq_len, dimension = tgt.size(1), tgt.size(2)
  tgt += position_encoding(seq_len, dimension)
  for layer in self.layers:
    tgt = layer(tgt, memory)
  return torch.softmax(self.linear(tgt), dim=-1)
```

32.4 Inference of Autoregressive Model

In an autoregressive transformer (such as GPT), tokens are generated one at a time. During inference, the model must compute attention for the next token based on all previously generated tokens. However, because recomputing the entire attention from scratch at each time step would be inefficient, these models use *caching* to store intermediate results (the keys and values) from previous time steps. Below is an explanation with equations and clear notations.

Inference Overview in Autoregressive Models

- Training: The model can process the entire sequence in parallel using masked self-attention. A mask (typically a triangular matrix) prevents tokens from "seeing" future tokens.
- Inference: The model generates one token at a time. At time step $t + 1$, it uses the already generated tokens $[x_1, x_2, \ldots, x_t]$ to compute the probability distribution for the next token.

To avoid recomputing keys and values for tokens $x_1, \ldots, x_t$ at every step, the model stores them (usually for each layer). When a new token is generated, only its query needs to be computed, and then the cached keys and values are used to compute the attention.

The technique of storing and reusing the computed keys and values from previous tokens during autoregressive generation is commonly called *KV caching* (short for Key-Value Caching).

Step 1: Previous Tokens and Cached Representations Assume that by time step t the model has generated tokens:

$$x_1, x_2, \ldots, x_t.$$

For a given transformer layer, let the cached key and value matrices be:

$$K_{\leq t} \in \mathbb{R}^{t \times d_k},$$
$$V_{\leq t} \in \mathbb{R}^{t \times d_v},$$

where d_k is the key (and query) dimension and d_v is the value dimension.

Step 2: Compute the Query for the New Token When generating the next token x_{t+1}, its input (often the embedding of the previously generated token or a special "start" symbol) is used to compute a query vector for each layer:

$$q_{t+1} \in \mathbb{R}^{d_k}.$$

This is computed by a linear projection:

$$q_{t+1} = x_{t+1} W^Q,$$

where $W^Q \in \mathbb{R}^{d_{\text{model}} \times d_k}$ is the learned projection matrix.

Step 3: Compute the Attention Scores The new query q_{t+1} is compared with all the cached keys. In a single attention head, the (scaled) dot-product attention scores are computed as:

$$s_{t+1,j} = \frac{q_{t+1} \cdot k_j}{\sqrt{d_k}} \quad \text{for } j = 1, 2, \ldots, t,$$

and often, for implementation convenience, the new token's own key k_{t+1} is also computed and appended to the cache. In that case, you would have:

$$s_{t+1,j} = \frac{q_{t+1} \cdot k_j}{\sqrt{d_k}} \quad \text{for } j = 1, 2, \ldots, t+1.$$

Since the model is autoregressive, the mask is implicit. There are no "future" tokens beyond $t+1$ at inference time. (If you do compute for all $t+1$ positions, a mask would ensure that token $t+1$ only attends to tokens 1 through $t+1$.)

Step 4: Apply the Softmax to Get Attention Weights The scores are then normalized with the softmax function to obtain the attention weights:

$$\alpha_{t+1,j} = \frac{\exp(s_{t+1,j})}{\sum_{j'=1}^{t+1} \exp(s_{t+1,j'})}, \quad j = 1, \ldots, t+1.$$

These weights determine how much the new token attends to each of the previous tokens (and its own representation, if included).

Step 5: Compute the Weighted Sum of Values The output of the attention layer for the new token is then computed as:

$$z_{t+1} = \sum_{j=1}^{t+1} \alpha_{t+1,j}\, v_j,$$

where each v_j is the value vector from the cache (or computed for the new token in the case of $j = t+1$):

$$v_j = x_j\, W^V, \quad j = 1, \ldots, t+1.$$

This z_{t+1} is then passed on through the rest of the transformer layer (including feed-forward sub-layers, layer normalization, etc.) to eventually produce logits over the vocabulary.

Step 6: Generate the Next Token and Update the Cache

- The model uses the final output (after all transformer layers) to compute a probability distribution over the vocabulary.
- A token is chosen (*e.g.,* via sampling or greedy decoding) and appended to the sequence.
- The new token's key and value vectors (from each layer) are computed and added to the cache so that future tokens can attend to it.

32.4.1 Inference without Caching

Let's take a look at the following example:

- Number of tokens so far: $t = 3$. We have already generated tokens $\{x_1, x_2, x_3\}$. We now want to generate token x_4.
- Model dimensionality: To keep it simple, let's say each token embedding is 2-dimensional ($d_{\text{model}} = 2$) and the attention uses a single head with key/query dimension $d_k = 2$ and value dimension $d_v = 2$.
- Token embeddings (just made-up numbers):

  $$x_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad x_2 = \begin{bmatrix} 3 \\ 4 \end{bmatrix}, \quad x_3 = \begin{bmatrix} 5 \\ 6 \end{bmatrix}, \quad x_4 = \begin{bmatrix} ? \\ ? \end{bmatrix}$$

  The forth one is the one we want to generate. We will compute attention for tokens x_1, x_2, x_3, x_4 all at once.

- Projection matrices (W^Q, W^K, W^V) are each 2×2 for this example. For instance, we have the following matrices:

$$W^Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad W^K = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}, \quad W^V = \begin{bmatrix} 0.5 & -0.5 \\ 1.0 & 0.5 \end{bmatrix}.$$

Step A: Compute Queries, Keys, and Values

- Queries:

$$q_i = x_i \, W^Q$$

  For $i = 1, 2, 3, 4$:

  - $q_1 = [1 \;\; 2] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 \end{bmatrix}$
  - $q_2 = [3 \;\; 4] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 4 \end{bmatrix}$
  - $q_3 = [5 \;\; 6] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 6 \end{bmatrix}$
  - $q_4 = [?, \; ?] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} ? & ? \end{bmatrix}$

- Keys:

$$k_i = x_i \, W^K$$

  For $i = 1, 2, 3, 4$:

  - $k_1 = [1 \;\; 2] \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 4 \end{bmatrix}$
  - $k_2 = [3 \;\; 4] \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 10 \end{bmatrix}$
  - $k_3 = [5 \;\; 6] \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 16 \end{bmatrix}$
  - $k_4 = [?, \; ?] \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} ? & ? \end{bmatrix}$

- Values:

$$v_i = x_i \, W^V$$

  For $i = 1, 2, 3, 4$:

  - $v_1 = [1 \;\; 2] \begin{bmatrix} 0.5 & -0.5 \\ 1.0 & 0.5 \end{bmatrix} = \begin{bmatrix} 2.5 & 0.5 \end{bmatrix}$
  - $v_2 = [3 \;\; 4] \begin{bmatrix} 0.5 & -0.5 \\ 1.0 & 0.5 \end{bmatrix} = \begin{bmatrix} 5.5 & 0.5 \end{bmatrix}$
  - $v_3 = [5 \;\; 6] \begin{bmatrix} 0.5 & -0.5 \\ 1.0 & 0.5 \end{bmatrix} = \begin{bmatrix} 8.5 & 0.5 \end{bmatrix}$

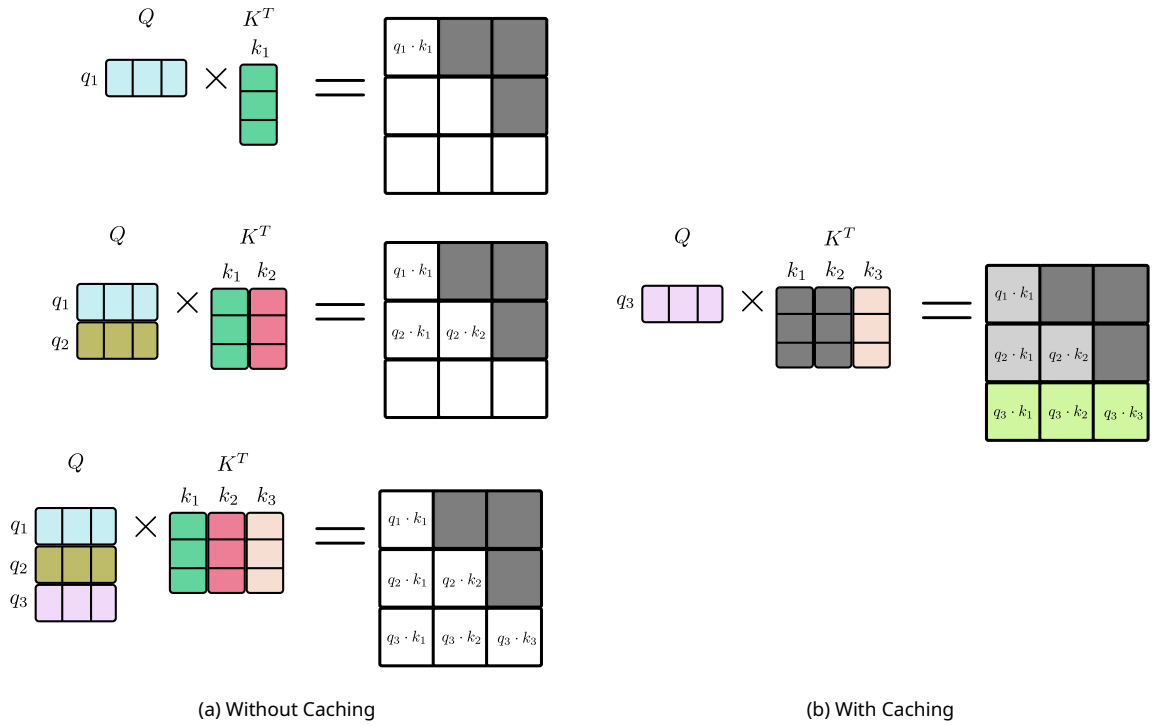


Figure 32.3: An example of KV caching

- $v_4 = [?,\ ?] \begin{bmatrix} 0.5 & -0.5 \\ 1.0 & 0.5 \end{bmatrix} = \begin{bmatrix} ? & ? \end{bmatrix}$

All of the above must be computed at the current time step if we do not use caching.

With KV caching, you would *not* recalculate k_1, k_2, k_3 and v_1, v_2, v_3. Instead:

- You already have $\{k_1, k_2, k_3\}$ and $\{v_1, v_2, v_3\}$ stored from the previous steps.
- You only compute:
  - q_4 (the query for the new token),
  - k_4, v_4 (the new key and value to add to the cache).

In other words, you skip re-projecting and re-computing every key and value from tokens $\{1, 2, 3\}$. This saves a substantial amount of computation when generating long sequences, especially in large transformers (like GPT).

Note that storing data in the cache uses up memory space. Systems with limited memory resources may struggle to accommodate this additional memory overhead, potentially resulting in out-of-memory errors. This is especially the case when long inputs need to be processed, as the memory required for the cache grows linearly with the input length and the batch size.

Computational Cost In sum, the vanilla self-attention on n tokens,

- each token needs to look at all n tokens to get attention scores

- Thus, the cost is $O(n^2)$

For instance, if we given a sentence with three tokens,

1. First token: Look at 1 token (cost: $O(1^2)$)
2. Second token: Look at 2 tokens (cost: $O(2^2)$)
3. Third token: Look at 3 tokens (cost: $O(3^2)$)

If we add up all these costs for generating a sequence of length n, we get:

$$O(1^2 + 2^2 + 3^2 + \cdots + n^2) \approx O(n^3)$$

With caching,

1. Process 1 token cost $O(1)$
2. Process 1 new token + look at 1 cached token cost $O(2)$
3. Process 1 new token + look at 2 cached tokens cost $O(3)$

Adding these up:

$$O(1 + 2 + 3 + \cdots + n) = O(n^2)$$

Chapter 33

Retrieval Augmented Generation

33.1 Introduction

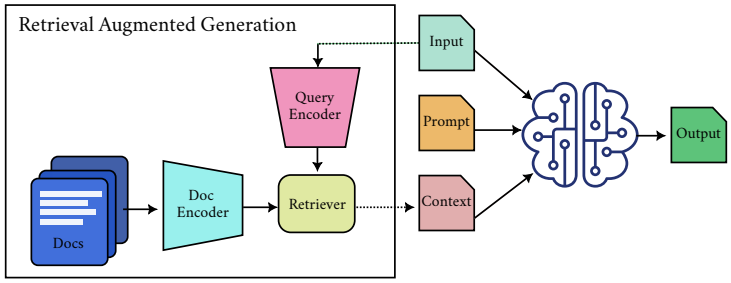


Figure 33.1: An overview of retrieval augmented generation.

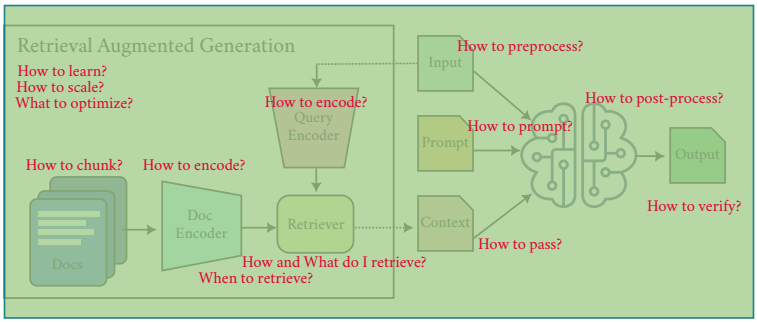


Figure 33.2: Open questions of RAG.

Chapter 34

Alignment Problems

34.1 Direct Preference Optimization

In RL, the goal is to train an agent to maximize a reward signal. However, in many real-world scenarios, the reward function is not explicitly known or is difficult to define. Instead, we often have access to preference data, where humans provide comparisons between different outputs or trajectories (*e.g.,* "Output A is better than Output B").

Traditional approaches to this problem involve:

- Learning a reward function from preference data.
- Using the learned reward function to train a policy via RL.

DPO simplifies this process by directly optimizing the policy to align with the preference data, bypassing the need for an explicit reward function. DPO can be represented as follows:

$$\mathcal{L}_{\text{DPO}}(\pi_\theta; \pi_{\text{ref}}) = -\mathbb{E}_{(x,y_w,w_l)\sim\mathcal{D}}\left[\log\sigma\left(\beta\log\frac{\pi_\theta(y_w|x)}{\pi_{\text{ref}}(y_w|x)} - \beta\log\frac{\pi_\theta(y_l|x)}{\pi_{\text{ref}}(y_l|x)}\right)\right], \tag{34.1}$$

where

- π_{ref} represents a *reference policy* (*e.g.,* a pre-trained or baseline policy).
- π_θ represents the *learned policy* parameterized by θ.

Let's deep dive into this equation. DPO leverages the *Bradley-Terry model*, a probabilistic framework for pairwise comparisons, to directly optimize the policy. The key idea is to express the probability of one output being preferred over another in terms of the policy's action probabilities. This allows the policy to be trained directly on preference data.

Assume that we have a dataset $\mathcal{D} = \{(x_i, y_i^1, y_i^2, p_i)\}_{i=1}^N$, where:

- x_i: Input context.
- y_i^1, y_i^2: Two possible outputs (*e.g.,* text responses or actions).

- p_i: Preference label, where $p_i = 1$ if y_i^1 is preferred over y_i^2, and $p_i = 0$ otherwise.

The Bradley-Terry model defines the probability that y_i^1 is preferred over y_i^2 as:

$$P(y_i^1 \succ y_i^2 \mid x_i) = \frac{\exp(r(x_i, y_i^1))}{\exp(r(x_i, y_i^1)) + \exp(r(x_i, y_i^2))},$$

where $r(x, y)$ is a reward function.

In DPO, the reward function $r(x, y)$ is parameterized by the learned policy $\pi_\theta(y \mid x)$ and the reference policy π_{ref}:

$$r(x, y) = \beta \log \frac{\pi_\theta(y \mid x)}{\pi_{\text{ref}}(y \mid x)},$$

where:

- β: A temperature parameter controlling the sharpness of the policy.
- $\pi_\theta(y \mid x)$: The probability of output y under the learned policy.
- $\pi_{\text{ref}}(y \mid x)$: The probability of output y under the reference policy.

This formulation ensures that the reward is tied to how much the learned policy π_θ deviates from the reference policy π_{ref}.

```
import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import DataLoader, Dataset
import numpy as np

# Set random seed for reproducibility
torch.manual_seed(42)
np.random.seed(42)

# Define a simple neural network for the policy
class PolicyNetwork(nn.Module):
    def __init__(self, input_dim, output_dim):
        super(PolicyNetwork, self).__init__()
        self.fc = nn.Sequential(
            nn.Linear(input_dim, 128),
            nn.ReLU(),
            nn.Linear(128, output_dim),
            nn.Softmax(dim=-1)  # Output is a probability distribution
        )

    def forward(self, x):
        return self.fc(x)

# Synthetic dataset for preference data
class PreferenceDataset(Dataset):
    def __init__(self, num_samples, input_dim):
        self.num_samples = num_samples
        self.input_dim = input_dim
        self.x = torch.randn(num_samples, input_dim)  # Random input contexts
        self.y1 = torch.randint(0, 2, (num_samples,))  # Random output 1
        self.y2 = torch.randint(0, 2, (num_samples,))  # Random output 2
        self.p = torch.randint(0, 2, (num_samples,))  # Random preferences (0
    or 1)

```

```
    def __len__(self):
        return self.num_samples

    def __getitem__(self, idx):
        return self.x[idx], self.y1[idx], self.y2[idx], self.p[idx]

# DPO loss function
def dpo_loss(pi_theta, pi_ref, y1, y2, p, beta=1.0):
    # Compute log probabilities under the learned and reference policies
    log_pi_theta_y1 = torch.log(pi_theta.gather(1, y1.unsqueeze(1))).squeeze()
    log_pi_theta_y2 = torch.log(pi_theta.gather(1, y2.unsqueeze(1))).squeeze()
    log_pi_ref_y1 = torch.log(pi_ref.gather(1, y1.unsqueeze(1))).squeeze()
    log_pi_ref_y2 = torch.log(pi_ref.gather(1, y2.unsqueeze(1))).squeeze()

    # Compute the reward differences
    r_y1 = beta * (log_pi_theta_y1 - log_pi_ref_y1)
    r_y2 = beta * (log_pi_theta_y2 - log_pi_ref_y2)

    # Compute the preference probability using the Bradley-Terry model
    logits = r_y1 - r_y2
    loss = -torch.mean(p * torch.log(torch.sigmoid(logits)) + (1 - p) * torch.log(torch.sigmoid(-logits)))
    return loss

# Hyperparameters
input_dim = 10  # Dimension of input context
output_dim = 2  # Number of possible outputs (binary for simplicity)
num_samples = 1000  # Number of preference pairs
batch_size = 32
learning_rate = 1e-3
num_epochs = 10
beta = 1.0  # Temperature parameter

# Create dataset and dataloader
dataset = PreferenceDataset(num_samples, input_dim)
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)

# Initialize policies
pi_theta = PolicyNetwork(input_dim, output_dim)  # Learned policy
pi_ref = PolicyNetwork(input_dim, output_dim)  # Reference policy (fixed)
pi_ref.eval()  # Freeze the reference policy

# Optimizer
optimizer = optim.Adam(pi_theta.parameters(), lr=learning_rate)

# Training loop
for epoch in range(num_epochs):
    for x, y1, y2, p in dataloader:
        # Forward pass: compute probabilities under the learned and reference policies
        pi_theta_probs = pi_theta(x)
        with torch.no_grad():
            pi_ref_probs = pi_ref(x)

        # Compute DPO loss
        loss = dpo_loss(pi_theta_probs, pi_ref_probs, y1, y2, p, beta)

        # Backward pass and optimization
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

    print(f"Epoch [{epoch+1}/{num_epochs}], Loss: {loss.item():.4f}")
```

```
96
97 # Test the learned policy
98 test_x = torch.randn(1, input_dim)  # Random test input
99 pi_theta_probs = pi_theta(test_x)
100 print(f"Test input: {test_x}")
101 print(f"Learned policy probabilities: {pi_theta_probs}")
```

Part VI

Advanced Topics

Chapter 35

Neural Ordinary Differential Equations

35.1 Preliminary

35.1.1 Euler Method

The Euler method is a simple numerical technique used to solve ordinary differential equations (ODEs) of the form $\frac{dy}{dt} = f(t, y)$. It is an initial value problem where we seek to find the function $y(t)$ given an initial condition $y(t_0) = y_0$. Here's a step-by-step explanation of the Euler method:

Problem Setup: Given,

- A differential equation $\frac{dy}{dt} = f(t, y)$
- An initial condition $y(t_0) = y_0$

Discretization: The idea is to approximate the solution at discrete points. Let's denote:

- t_n as the n-th time step
- y_n as the approximation of $y(t_n)$

We define a step size h such that $t_{n+1} = t_n + h$.

Euler's Approximation: Using the first-order Taylor series expansion, we can approximate $y(t)$ at t_{n+1} as:

$$y_{n+1} \approx y_n + h \cdot f(t_n, y_n)$$

Iterative Process: Starting from the initial condition (t_0, y_0):

1. Calculate the next value using the formula:
$$y_{n+1} = y_n + h \cdot f(t_n, y_n)$$
2. Repeat the process for $n = 0, 1, 2, \ldots$ until the desired value of t is reached.

Example: Let's solve the differential equation $\frac{dy}{dt} = y$ with the initial condition $y(0) = 1$ using the Euler method.

- Set the step size h (e.g., $h = 0.1$).
- Start with $t_0 = 0$ and $y_0 = 1$.

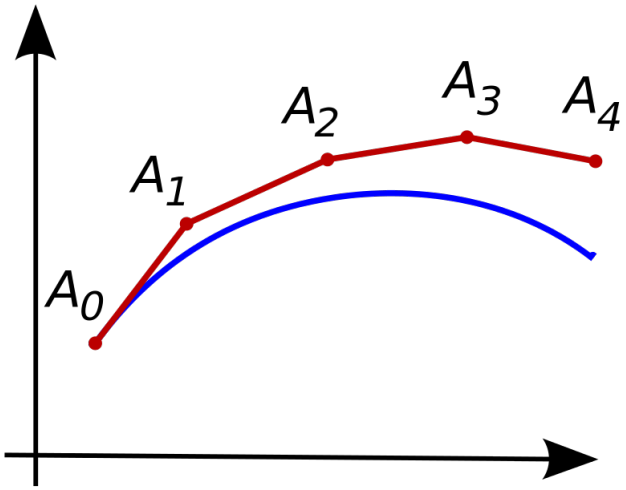
Using the Euler formula:

$$y_1 = y_0 + h \cdot f(t_0, y_0) = 1 + 0.1 \cdot 1 = 1.1$$

$$y_2 = y_1 + h \cdot f(t_1, y_1) = 1.1 + 0.1 \cdot 1.1 = 1.21$$

$$y_3 = y_2 + h \cdot f(t_2, y_2) = 1.21 + 0.1 \cdot 1.21 = 1.331$$

Euler's method can be visualized as taking small steps along the curve defined by the differential equation, using the slope at the current point to determine the direction of the next step.



Advantages:

- Simple to understand and implement.
- Requires only basic arithmetic operations.

Disadvantages:

- Low accuracy for large step sizes.
- Can become unstable if the step size is not chosen appropriately.
- Errors accumulate over time, leading to less accurate solutions.

Euler's method is often used as a basic introduction to numerical methods for solving ODEs, and more sophisticated methods like the *Runge-Kutta* methods are used for more accurate solutions.

35.2 Neural ODE

Models such as residual networks, recurrent neural network decoders, and normalizing flows build complicated transformations by composing a sequence of transformations to a hidden state:

$$\mathbf{h}_{t+1} = \mathbf{h}_t + f(\mathbf{h}_t, \theta_t).$$

The $\mathbf{h}$ is iteratively updated as follows:

$$\begin{aligned}
\mathbf{h}_2 &= \mathbf{h}_1 + f(\mathbf{h}_1, \theta) \\
\mathbf{h}_3 &= \mathbf{h}_2 + f(\mathbf{h}_2, \theta) = \mathbf{h}_1 + f(\mathbf{h}_1, \theta) + f(\mathbf{h}_2, \theta) \\
&\vdots
\end{aligned}$$

These iterative update can be seen as *Euler discretization* of the *continuous* transformation. Think of traditional neural networks as a sequence of steps. You give it some input, it goes through several steps (layers), and you get an output. Instead of thinking in steps, Neural ODEs think in **continuous change over time**. Note that this is the key contribution of this approach.

Euler method can be expressed as follows:

$$y_n = y_{n-1} + h\frac{\partial y_{n-1}}{\partial x_{n-1}},$$

where h is the step size. In NODE, they view the f as an ordinary differential equation, which depends on the state at time t and parameter θ. The following equation is the shape of Euler method:

$$y_n = y_1 + h\frac{\partial y_1}{\partial x_1} + h\frac{\partial y_2}{\partial x_2} + \cdots + h\frac{\partial y_{n-1}}{\partial x_{n-1}}.$$

In NODE,

Chapter 36

State Estimations

36.1 Introduction to State-Space Model

Reference: State-Space Models.

A state-space model is a mathematical framework used to describe a system by a set of input, output, and state variables related by first-order differential (or difference) equations. It's widely used in control theory, signal processing, and time series analysis.

For a continuous-time system, the state-space model is typically expressed as follows:

$$\dot{x}(t) = Ax(t) + Bu(t),$$
$$y(t) = Cx(t) + Du(t).$$

The first and the second equations are known as *state equation* and *output equation*, respectively. The state equation tells us that how the state vector changes with the state vector and the (external) input. The state space model is **linear** and **time invariant**, since the equations are linear and the parameter matrices do not change over time. Such systems are referred as a LTI system.

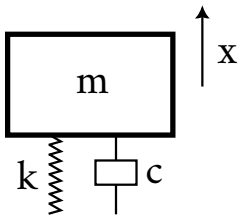
- $x(t) \in \mathbb{R}^n$: A state vector. This variable describes the state of the system at any given time.
- $\dot{x} \in \mathbb{R}^n$: state derivative *i.e.,* $\left(\frac{dX}{dt}\right)$ represents the changes of the state vector. You can notice that this is a linear combination of state vector and the input vector.
- $u \in \mathbb{R}^m$: An external input affecting the system.
- $y \in \mathbb{R}^p$: An (Observed) Output.
- $A \in \mathbb{R}^{n \times n}$: A state matrix. This matrix describes how the state vector influences the changes of the state vector.
- $B \in \mathbb{R}^{n \times m}$: An input matrix. This matrix describes how the (external) input vector influences the changes of the state vector.
- $C \in \mathbb{R}^{p \times n}$: An output matrix. Typically, an identity matrix (I).
- $D \in \mathbb{R}^{p \times m}$: A feedthrough (or direct transmission) matrix. Typically, zeros

36.1.1 Example: Mass-Spring-Damper System

Let's consider a simple example of a mass-spring-damper system, which can be described by the second-order differential equation.

The mass-spring-damper system is a common mechanical system that consists of three main components:

- Mass (m): A mass that can move along a straight line.
- Spring (k): A spring that exerts a force proportional to its displacement from its equilibrium position (Hooke's Law).
- Damper (c): A damping element (like a shock absorber) that exerts a force proportional to the velocity of the mass (damping force).



System Dynamics The dynamics of this system can be described by Newton's second law of motion, which states that the sum of forces acting on the mass is equal to the mass times its acceleration ($F = ma$).

Differential Equation For a mass-spring-damper system, the forces are:

- Spring Force: $F_{\text{spring}} = -kx(t)$, where $x(t)$ is the displacement of the mass from its equilibrium position. The proportional constant k is called the spring constant. It is a measure of the spring's stiffness.
- Damping Force: Damping forces are a special type of force that are used to slow down or stop a motion. $F_{\text{damper}} = -c\dot{x}(t)$, where $\dot{x}(t)$ is the velocity of the mass (or object). Note that $\dot{x}(t) = dx(t)/dt$.
- External Force: $F(t)$, an external force applied to the mass.

By summing these forces, we get:

$$m\ddot{x}(t) = -kx(t) - c\dot{x}(t) + F(t).$$

To explain, the external force is stretching the spring, and the damper and the spring force are pulling the mass. Rearranging this, we get the second-order differential equation:

$$m\ddot{x}(t) + c\dot{x}(t) + kx(t) = F(t)$$

State-Space Representation To convert this second-order differential equation into a state-space representation, we need to express it as a system of first-order differential equations.

Defining State Variables We introduce two state variables:

- $x_1(t) = x(t)$: the position of the mass.
- $x_2(t) = \dot{x}(t)$: the velocity of the mass.

Now, we can write the original second-order equation as two first-order equations:

$$\dot{x}_1(t) = x_2(t)$$

$$\dot{x}_2(t) = \frac{1}{m}F(t) - \frac{k}{m}x_1(t) - \frac{c}{m}x_2(t)$$

Matrix Form We can express these equations in matrix form:

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{m} \end{bmatrix} F(t)$$

This is the state-space form:

$$\dot{x}(t) = Ax(t) + Bu(t)$$

Where:

- $x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}$ is the state vector.
- $u(t) = F(t)$ is the input (external force).
- $A = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix}$ is the state matrix.
- $B = \begin{bmatrix} 0 \\ \frac{1}{m} \end{bmatrix}$ is the input matrix.

Output Equation If we consider the output to be the position of the mass ($x_1(t)$), the output equation is:

$$y(t) = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}$$

So, the output equation is:

$$y(t) = Cx(t),$$

Where $C = \begin{bmatrix} 1 & 0 \end{bmatrix}$.

Full State-Space Model Combining the state and output equations, we get the full state-space representation:

$$\dot{x}(t) = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix} x(t) + \begin{bmatrix} 0 \\ \frac{1}{m} \end{bmatrix} u(t)$$
$$y(t) = \begin{bmatrix} 1 & 0 \end{bmatrix} x(t)$$

In sum,

- State variables: $x_1(t) = x(t)$ (position), $x_2(t) = \dot{x}(t)$ (velocity)
- Input: $u(t) = F(t)$ (external force)
- Output: $y(t) = x(t)$ (position)
- State equation: $\dot{x}(t) = Ax(t) + Bu(t)$
- Output equation: $y(t) = Cx(t)$

This state-space model describes how the position and velocity of the mass change over time in response to an external force.

36.1.2 Stability

The linear state space model is stable if all eigenvalues of A are negative real numbers or have negative real parts to complex number eigenvalues. If all real parts of the eigenvalues are negative then the system is stable, meaning that any initial condition converges exponentially to a stable attracting point. If any real parts are zero then the system will not converge to a point and if the eigenvalues are positive the system is unstable and will exponentially diverge.

Chapter 37

Kalman Filter

37.1 Propagation of States and Covariances

Suppose we have a linear discrete-time system:

$$\boldsymbol{\theta}_k = F_{k-1}\boldsymbol{\theta}_{k-1} + G_{k-1}\mathbf{u}_{k-1} + \mathbf{w}_{k-1},$$

where $\mathbf{w}_k$ is a Gaussian zero-mean white noise with covariance Q_k and $\mathbf{u}_k$ is a known input. The F and G are state and input matrices, respectively. How does the mean of the state $\boldsymbol{\theta}_k$ changes over time? The expectation is given by

$$\mathbb{E}[\boldsymbol{\theta}_k] = \mathbb{E}[F_{k-1}\boldsymbol{\theta}_{k-1}] + \mathbb{E}[G_{k-1}\mathbf{u}_{k-1}] + \mathbb{E}[\mathbf{w}_{k-1}]$$

For simplicity, we can write it as

$$\overline{\boldsymbol{\theta}}_k = F_{k-1}\overline{\boldsymbol{\theta}}_{k-1} + G_{k-1}\mathbf{u}_{k-1}.$$

How does the state covariance of $\boldsymbol{\theta}_k$ change with time? The state covariance matrix propagation is given by

$$P_k = \mathbb{E}[(\boldsymbol{\theta}_k - \overline{\boldsymbol{\theta}}_k)(\boldsymbol{\theta}_k - \overline{\boldsymbol{\theta}}_k)^T]$$

and then compute the expectation of every term in that expression.

$$\begin{aligned}(\boldsymbol{\theta}_k - \overline{\boldsymbol{\theta}}_k)(\boldsymbol{\theta}_k - \overline{\boldsymbol{\theta}}_k)^T &= (F_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1}) + \mathbf{w}_{k-1})(F_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1}) + \mathbf{w}_{k-1})^T \\ &= F_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})^T F_{k-1}^T + F_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})\mathbf{w}_{k-1}^T \\ &+ \mathbf{w}_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})^T F_{k-1}^T + \mathbf{w}_{k-1}\mathbf{w}_{k-1}^T\end{aligned}$$

Since $(\boldsymbol{\theta}_k - \overline{\boldsymbol{\theta}}_k)$ is uncorrelated to $\mathbf{w}_{k-1}$, we have

$$\begin{aligned}E[F_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})\mathbf{w}_{k-1}^T] = 0 \\ E[\mathbf{w}_{k-1}(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})^T F_{k-1}^T] = 0\end{aligned}$$

Also, we have

$$E[\mathbf{w}_{k-1}\mathbf{w}_{k-1}^T] = Q_{k-1}$$

$$P_{k-1} = E[(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})(\boldsymbol{\theta}_{k-1} - \overline{\boldsymbol{\theta}}_{k-1})^T]$$

By using these expressions, we obtain the final equation for the propagation of the state covariance matrix

$$P_k = F_{k-1}P_{k-1}F_{k-1}^T + Q_{k-1}$$

This is called a discrete time *Lyapunov equation*, or a *Stein equation*. It is interesting to consider the conditions under which the discrete time Lyapunov equation has a *steady-state solution*.

37.2 Kalman Filtering

We are considering the following state-space model of a dynamical system:

$$\begin{aligned}\boldsymbol{\theta}_k &= F_{k-1}\boldsymbol{\theta}_{k-1} + G_{k-1}\mathbf{u}_{k-1} + \mathbf{w}_{k-1}\\ \mathbf{y}_k &= \mathbf{X}_k\boldsymbol{\theta}_k + \boldsymbol{\eta}_k,\end{aligned}$$

where

- $\mathbf{w}_k \sim (0, Q_k)$: process noise vector
- $E[\mathbf{w}_k\mathbf{w}_j^T] = Q_k\delta_{k-j}$
- $\boldsymbol{\eta}_k \sim (0, R_k)$: measurement noise vector
- $E[\boldsymbol{\eta}_k\boldsymbol{\eta}_j^T] = R_k\delta_{k-j}$
- $E[\boldsymbol{\eta}_k\mathbf{w}_j^T] = 0$
- $\mathbf{u}_{k-1}$: control unit vector
- F and G are state and input matrices.

Our primary goal is to estimate the state $\boldsymbol{\theta}_k$ based on our knowledge of the system dynamics and the availability of the noisy measurements $\mathbf{y}_k$.

If we have all of the measurements up to and including time k available for use in our estimate of $\boldsymbol{\theta}_k$, then we can form an a *posteriori estimate*, which we denote as $\hat{\boldsymbol{\theta}}_k^+$. The + superscript denotes that the estimate is a posteriori. One way to form the a posteriori state estimate is to compute the expected value of $\boldsymbol{\theta}_k$ conditioned on a ll of the measurements up to and including time k:

$$\hat{\boldsymbol{\theta}}_k^+ = E[\boldsymbol{\theta}_k|\mathbf{y}_1, \ldots, \mathbf{y}_{k-1}, \mathbf{y}_k].$$

If we have all of the measurements before (but not including) time k available for use in our estimate of $\boldsymbol{\theta}_k$, then we can form an a praori estimate, which we denote

$$\hat{\boldsymbol{\theta}}_k^-.$$

One way to form the a *priori state estimate* is to compute the expected value of $\boldsymbol{\theta}_k$, conditioned on all of the measurements before (but not including) time k:

$$\hat{\boldsymbol{\theta}}_k^- = E[\boldsymbol{\theta}_k|\mathbf{y}_1, \ldots, \mathbf{y}_{k-1}].$$

By their nature, it is natural to expect that $\hat{\boldsymbol{\theta}}_k^+$ to be a better estimate than $\hat{\boldsymbol{\theta}}_k^-$, since we can leverage more information to compute it.

If we have measurements after time k available for use in our estimate of $\boldsymbol{\theta}_k$, then we can form a *smoothed estimate*. One way to form the smoothed state estimate is to compute the expected value of $\boldsymbol{\theta}_k$ conditioned on all of the measurements that are available:

$$\hat{\boldsymbol{\theta}}_{k|k+N} = E[\boldsymbol{\theta}_k|\mathbf{y}_1, \ldots, \mathbf{y}_k, \ldots, \mathbf{y}_{k+N}],$$

where N is some positive integer. If we want to find the best prediction of $\boldsymbol{\theta}_k$ more than one time step ahead of the available measurements, then we can form a predicted estimate. One way to form the *predicted state estimate* is to compute the expected value of $\boldsymbol{\theta}_k$ conditioned on all of the measurements that are available:

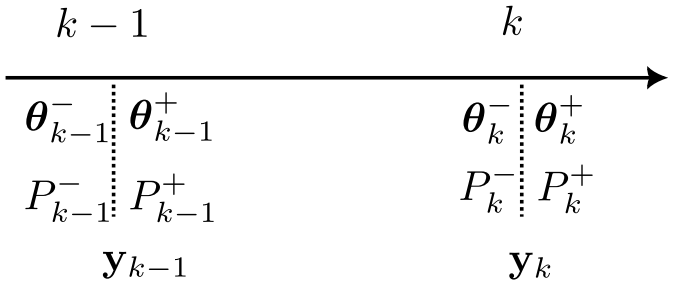
$$\hat{\boldsymbol{\theta}}_{k|k-M} = E[\boldsymbol{\theta}_k|\mathbf{y}_1, \ldots, \mathbf{y}_{k-M}].$$

The relationship between the a posteriori, a priori, smoothed, and predicted state estimates is represented in the following figure:

As done in RLS (*c.f.,* §10.1), we should define covariance matrices of the a priori and the a posteriori estimation errors. The covariance matrices are defined as follows:

$$P_k^- = \mathbb{E}[(\boldsymbol{\theta}_k - \boldsymbol{\theta}_k^-)(\boldsymbol{\theta}_k - \boldsymbol{\theta}_k^-)^T]$$
$$P_k^+ = \mathbb{E}[(\boldsymbol{\theta}_k - \boldsymbol{\theta}_k^+)(\boldsymbol{\theta}_k - \boldsymbol{\theta}_k^+)^T],$$

where P_k^- is the covariance matrix of the a priori estimation error and P_k^+ is the covariance matrix of the a posteriori estimation error.



After the discrete-time instant $k-1$, we compute the a posteriori state estimate $\boldsymbol{\theta}_{k-1}^+$ and the covariance matrix of the estimation error P_{k-1}^+. Then, we propagate these quantities through the equations describing the system dynamics and covariance matrix propagation (that is also derived on the basis of the system dynamics). That is, we propagate the a posteriori state and covariance through our model. By propagating these quantities, we obtain the a priori state estimate $\boldsymbol{\theta}_k^-$ and the covariance matrix of the estimation error P_k^- for the time step k. Then, after the measurement vector $\mathbf{y}_k$ is observed at the discrete-time step k, we use this measurement and the recursive-least squares method to compute the a posteriori estimate $\boldsymbol{\theta}_k^+$ and the covariance matrix of the estimation error P_k^+ for the time instant k.

This is how Kalman filter works. Now let's derive the equations of Kalman filter. At the initial time instant $k = 0$, we need to set an initial guess of the state estimate, $\hat{\boldsymbol{\theta}}_0$. This will be our initial a posteriori state estimate, that is

$$\hat{\boldsymbol{\theta}}_0^+ = \hat{\boldsymbol{\theta}}_0$$

Then, the question is how to compute the a priori estimate $\hat{\boldsymbol{\theta}}_1^-$ at $k = 1$. The natural answer is that the system states, as well as the estimates, need to satisfy the system dynamics (1), and consequently,

$$\hat{\boldsymbol{\theta}}_1^- = F_0\hat{\boldsymbol{\theta}}_0^+ + F_0\mathbf{u}_0$$

where we excluded the disturbance part since the disturbance vector is not known. Besides the initial guess of the estimate, we also need to select an initial guess of the covariance matrix of the estimation error. That is, we need to select P_0^+. If we have perfect knowledge about the initial state, then we select P_0^+ as a zero matrix, that is $P_0^+ = 0 \cdot I$, where I is an identity matrix. This is because the covariance matrix of the estimation error is the measure of uncertainty, and if we have perfect knowledge, then the measure of uncertainty should be zero. On the other hand, if we do not have any a priori knowledge of the initial state, then $P_0^+ = c \cdot I$, where c is a large number. Next, we need to compute the covariance matrix of the a priori state estimation error, that is, we need to compute P_1^-. In our previous post, which can be found here, we derived the expression for the time propagation of the covariance matrix of the state estimation error:

$$P_k = F_{k-1} P_{k-1} F_{k-1}^T + Q_{k-1}$$

By using this expression, we obtain the following equation forP_1^-.

37.2.1 Python Implementation

```
class KalmanFilter(object):

  # x0 - initial guess of the state vector
  # P0 - initial guess of the covariance matrix of the state estimation error
  # A,B,C - system matrices describing the system model
  # Q - covariance matrix of the process noise
  # R - covariance matrix of the measurement noise

  def __init__(self,x0,P0,A,B,C,Q,R):

      # initialize vectors and matrices
      self.x0=x0
      self.P0=P0
      self.A=A
      self.B=B
      self.C=C
      self.Q=Q
      self.R=R

      # this variable is used to track the current time step k of the
  estimator
      # after every measurement arrives, this variables is incremented for +1
      self.currentTimeStep=0

      # this list is used to store the a posteriori estimates xk^{+} starting
   from the initial estimate
      # note: list starts from x0^{+}=x0 - where x0 is an initial guess of
  the estimate
      self.estimates_aposteriori=[]
      self.estimates_aposteriori.append(x0)

      # this list is used to store the a apriori estimates xk^{-} starting
  from x1^{-}
      # note: x0^{-} does not exist, that is, the list starts from x1^{-}
      self.estimates_apriori=[]

      # this list is used to store the a posteriori estimation error
  covariance matrices Pk^{+}
      # note: list starts from P0^{+}=P0, where P0 is the initial guess of
  the covariance
      self.estimationErrorCovarianceMatricesAposteriori=[]
```

```
36          self.estimationErrorCovarianceMatricesAposteriori.append(P0)
37
38          # this list is used to store the a priori estimation error covariance
    matrices Pk^{-}
39          # note: list starts from P1^{-}, that is, P0^{-} does not exist
40          self.estimationErrorCovarianceMatricesApriori=[]
41
42          # this list is used to store the gain matrices Kk
43          self.gainMatrices=[]
44
45          # this list is used to store prediction errors error_k=y_k-C*xk^{-}
46          self.errors=[]
47
48      # this function propagates x_{k-1}^{+} through the model to compute x_{k
    }^{-}
49      # this function also propagates P_{k-1}^{+} through the covariance model to
         compute P_{k}^{-}
50      # at the end this function increments the time index currentTimeStep for +1
51      def propagateDynamics(self,inputValue):
52
53          xk_minus=self.A*self.estimates_aposteriori[self.currentTimeStep]+self.B
    *inputValue
54          Pk_minus=self.A*self.estimationErrorCovarianceMatricesAposteriori[self.
    currentTimeStep]*(self.A.T)+self.Q
55
56          self.estimates_apriori.append(xk_minus)
57          self.estimationErrorCovarianceMatricesApriori.append(Pk_minus)
58
59          self.currentTimeStep=self.currentTimeStep+1
60
61      # this function should be called after propagateDynamics() because the time
         step should be increased and states and covariances should be propagated
62      def computeAposterioriEstimate(self,currentMeasurement):
63          import numpy as np
64          # gain matrix
65          Kk=self.estimationErrorCovarianceMatricesApriori[self.currentTimeStep
    -1]*(self.C.T)*np.linalg.inv(self.R+self.C*self.
    estimationErrorCovarianceMatricesApriori[self.currentTimeStep-1]*(self.C.T))
66
67          # prediction error
68          error_k=currentMeasurement-self.C*self.estimates_apriori[self.
    currentTimeStep-1]
69          # a posteriori estimate
70          xk_plus=self.estimates_apriori[self.currentTimeStep-1]+Kk*error_k
71
72          # a posteriori matrix update
73          IminusKkC=np.matrix(np.eye(self.x0.shape[0]))-Kk*self.C
74          Pk_plus=IminusKkC*self.estimationErrorCovarianceMatricesApriori[self.
    currentTimeStep-1]*(IminusKkC.T)+Kk*(self.R)*(Kk.T)
75
76          # update the lists that store the vectors and matrices
77          self.gainMatrices.append(Kk)
78          self.errors.append(error_k)
79          self.estimates_aposteriori.append(xk_plus)
80          self.estimationErrorCovarianceMatricesAposteriori.append(Pk_plus)
```

Chapter 38

Deep State Space Models

38.1 Efficiently Modeling Long Sequences with Structured State-Spaces

The Linear State-Space Layer (LSSL) is a simple sequence model that maps a one-dimensional function or sequence $u(t) \to y(t)$ through an implicit state $x(t)$ by simulating a linear continuous-time state-space representation in discrete-time

$$\begin{aligned} x'(t) &= \mathbf{A}x(t) + \mathbf{B}u(t), \\ y(t) &= \mathbf{C}x(t) + \mathbf{D}u(t). \end{aligned}$$

The first equation maps a single dimensional input signal $u(t)$ (or sequence) to an N-dim latent state (or hidden state) $x'(t)$ with the current state $x(t)$. The $\mathbf{A}$ and $\mathbf{B}$ can be considered as an non-linear mapping or transition matrices (*i.e.,* learnable parameters) to reflect the impact of the current state and the input, respectively. Finally, we project the input and the updated state to a one-dim output signal $y(t)$ (*i.e.,* sequence).

Our goal is to simply use the SSM as a black-box representation in a deep sequence model, where $\mathbf{A}, \mathbf{B}, \mathbf{C}$, and $\mathbf{D}$ are parameters learned by gradient descent. We will omit the parameter $\mathbf{D}$ for exposition (or equivalently, assume $\mathbf{D} = 0$, because the term $\mathbf{D}u$ can be viewed as a *skip connection* that doesn't depend on the hidden state (x)).

An SSM maps a input $u(t)$ to a state representation vector $x(t)$ and an output $y(t)$. For simplicity, we assume the input and output are one-dimensional, and the state representation is N-dimensional. The first equation defines the change in $x(t)$ over time.

Discretization We want to find a discrete-time state-space model. We can represent it by approximating a continuous model (*i.e.,* $h(t_k) \approx h(k\Delta)$) as follows:

$$\begin{aligned} x'(t) &= \overline{\mathbf{A}}x(t) + \overline{\mathbf{B}}u(t), \\ y(t) &= \mathbf{C}x(t) + \underbrace{\mathbf{D}u(t)}_{=0}, \end{aligned}$$

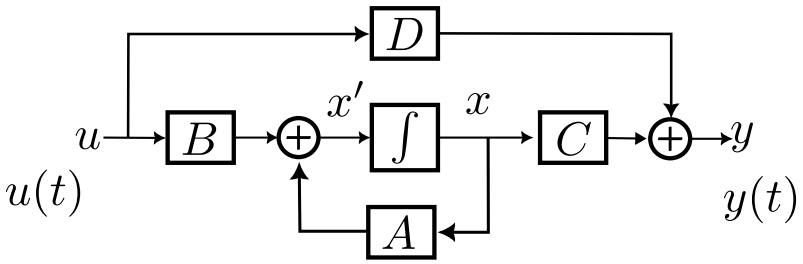


Figure 38.1: S4 Model

where $\overline{\mathbf{A}} = \mathbf{I} + \Delta\mathbf{A}$ and $\overline{\mathbf{B}} = \Delta\mathbf{B}$, respectively. They are derived by

$$\begin{aligned} x'(t) &= \overline{\mathbf{A}}x(t) + \overline{\mathbf{B}}u(t) \\ &= \lim_{\Delta \to 0} \frac{x(t+\Delta) - x(t)}{\Delta}, \end{aligned}$$

where Δ is a step size. Note that Δ is a learnable parameter to be determined during a training phase. Subsequently, we get

$$x(t+\Delta) - x(t) = \Delta x'(t).$$

Equivalently,

$$x(t+\Delta) = \Delta x'(t) + x(t).$$

Plugging $x'(t)$ into the above equation, we get:

$$\begin{aligned} x(t+\Delta) &= \Delta(\mathbf{A}x(t) + \mathbf{B}u(t)) + x(t) \\ &= \underbrace{(\mathbf{I} + \Delta\mathbf{A})}_{\overline{\mathbf{A}}} x(t) + \underbrace{\Delta\mathbf{B}}_{\overline{\mathbf{B}}} u(t). \end{aligned}$$

We can say $x(t+\Delta) = x(t+1)$, since it is the next state we care. Thus,

$$x(t+1) = (\mathbf{I} + \Delta\mathbf{A})x(t) + \Delta\mathbf{B}u(t).$$

Note that the original paper utilizes a special rule called *Zero-Order Hold* to approximate the $\overline{A}$ and $\overline{B}$.

Alternatively, we can use the trapezoidal method. The trapezoidal rule works by approximating the region under the graph of the function $f(x)$ as a trapezoid and calculating its area. It follows that

$$\int_a^b f(x)\,dx \approx (b-a) \cdot \tfrac{1}{2}(f(a) + f(b)).$$

Thus, the integral of $x'(t)$ from t_n to t_{n+1} can be approximated using the trapezoidal rule. The exact integral is:

$$\begin{aligned} x(t_{n+1}) - x(t_n) &= \int_{t_n}^{t_{n+1}} x'(t)dt \\ &\approx \frac{1}{2}\Delta(\mathbf{A}x(t_{n+1}) + \mathbf{B}u(t_{n+1}) + \mathbf{A}x(t_n) + \mathbf{B}u(t_n)), \end{aligned}$$

where $\Delta = t_{n+1} - t_n$. Then, we have

$$x(t_{n+1}) - \frac{\Delta}{2}\mathbf{A}x(t_{n+1}) = x(t_n) + \frac{\Delta}{2}\mathbf{A}x(t_n) + \frac{\Delta}{2}\mathbf{B}u(t_n) + \frac{\Delta}{2}\mathbf{B}u(t_{n+1})$$

$$\left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)x(t_{n+1}) = \left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)x(t_n) + \Delta\mathbf{B}\frac{(u(t_n) + u(t_{n+1})}{2}$$

$$x(t_{n+1}) = \left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)^{-1}\left(\mathbf{I} + \frac{\Delta}{2}\mathbf{A}\right)x(t_n) + \left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)^{-1}\frac{\Delta}{2}\mathbf{B}(u(t_{n+1}))$$

Finally, we get

$$\overline{\mathbf{A}} = \left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)^{-1}\left(\mathbf{I} + \frac{\Delta}{2}\mathbf{A}\right)$$
$$\overline{\mathbf{B}} = \left(\mathbf{I} - \frac{\Delta}{2}\mathbf{A}\right)^{-1}\Delta\mathbf{B}$$

Note that we assume that $u(t_{n+1}) \approx u(t_n)$. We can represent the update process as follows: At $t = 0$

$$x(0) = \overline{\mathbf{B}}u(0),$$
$$y(0) = \mathbf{C}x(0)$$

At $t = 1$

$$x(1) = \overline{\mathbf{A}}x(0) + \overline{\mathbf{B}}u(1),$$
$$y(1) = \mathbf{C}x(1)$$

At $t = 2$

$$x(2) = \overline{\mathbf{A}}x(1) + \overline{\mathbf{B}}u(2),$$
$$y(2) = \mathbf{C}x(2).$$

Note that this update process is equivalent to the RNN's update process.

As a Convolution The above process can be viewed as an one-dimensional convolution.

$$x(0) = \overline{\mathbf{B}}u(0),$$
$$y(0) = \mathbf{C}x(0) = \mathbf{C}\overline{\mathbf{B}}u(0)$$

$$x(1) = \overline{\mathbf{A}}x(0) + \overline{\mathbf{B}}u(1) = \overline{\mathbf{A}\mathbf{B}}u(0) + \overline{\mathbf{B}}u(1)$$
$$y(1) = \mathbf{C}x(1) = \mathbf{C}(\overline{\mathbf{A}\mathbf{B}}u(0) + \overline{\mathbf{B}}u(1)) = \mathbf{C}\overline{\mathbf{A}\mathbf{B}}u(0) + \mathbf{C}\overline{\mathbf{B}}u(1)$$

$$x(2) = \overline{\mathbf{A}}x(1) + \overline{\mathbf{B}}u(2) = \overline{\mathbf{A}}(\overline{\mathbf{A}\mathbf{B}}u(0) + \overline{\mathbf{B}}u(1)) + \overline{\mathbf{B}}u(2) = \overline{\mathbf{A}}^2\overline{\mathbf{B}}u(0) + \overline{\mathbf{A}\mathbf{B}}u(1) + \overline{\mathbf{B}}u(2)$$
$$y(2) = \mathbf{C}x(2) = \mathbf{C}(\overline{\mathbf{A}}^2\overline{\mathbf{B}}u(0) + \overline{\mathbf{A}\mathbf{B}}u(1) + \overline{\mathbf{B}}u(2)) = \mathbf{C}\overline{\mathbf{A}}^2\overline{\mathbf{B}}u(0) + \mathbf{C}\overline{\mathbf{A}\mathbf{B}}u(1) + \mathbf{C}\overline{\mathbf{B}}u(2)$$

We get a general formula:

$$\begin{aligned} y(t) &= \mathbf{C}\overline{\mathbf{A}}^t\overline{\mathbf{B}}u(0) + \mathbf{C}\overline{\mathbf{A}}^{t-1}\overline{\mathbf{B}}u(1) + \cdots + \mathbf{C}\overline{\mathbf{B}}u(t) \\ &= \sum_{t=0}^{T}\mathbf{C}\overline{\mathbf{A}}^{T-t}\overline{\mathbf{B}}u(t) \end{aligned}$$

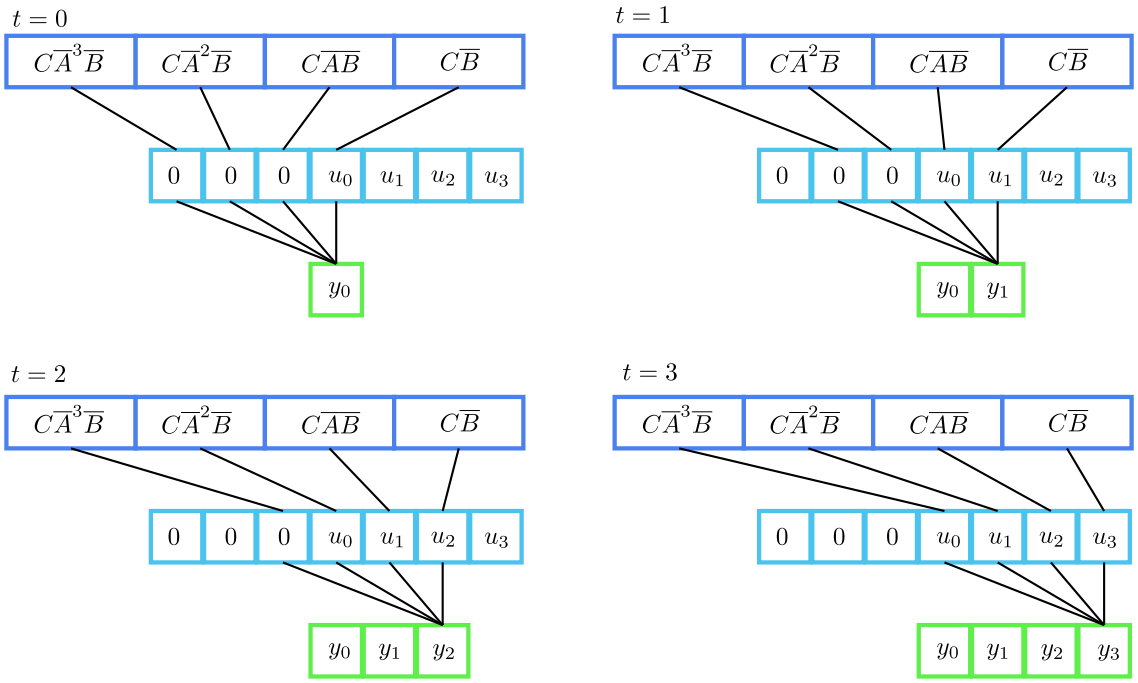


Figure 38.2:

It turns out that the above equation is a one-dimensional convolution by a kernel $\overline{\mathbf{K}}$:

$$y = x * \overline{\mathbf{K}}.$$

It is generally referred to as the SSM convolution kernel in the literature, and its size is equivalent to the entire input sequence. This convolution kernel is calculated by Fast Fourier Transform (FFT)

Let's say the kernel size is 4 with zero-padding, (See Fig. 38.2). During training, we can train the model as a convolutional neural network so that we can leverage the parallel training. During inference (*i.e.,* decoding stage), we can switch to the recurrent mode for near-constant time inference. Please note here, that if you look at the kernels you can see that they are fixed.

In the convolution kernel developed above, $\bar{\mathbf{C}}$ and $\bar{\mathbf{B}}$, are learnable scalars. Concerning $\bar{\mathbf{A}}$, we've seen that in our convolution kernel, it's expressed as a power of k at time k. This can be very time-consuming to calculate, so we're looking for a fixed $\bar{\mathbf{A}}$. For this, the best option is to have it diagonal:

Note that we can scale the single-dimensional SSM to multi-dimensional vector by putting a SSM for each dimension. For instance, there is going to be 256 SSMs if we want to learn a 256 embeddings.

38.2 Mamba: Linear-Time Sequence Modeling with Selective State Spaces

https://blog.premai.io/s4-and-mamba/

We can immediately notice the importance of the matrix $\mathbf{A}$. The Mamba leverages a special matrix called HiPPO. The HiPPO is a NxN matrix specifically designed to approximate all the

input signals by using Legendre polynomials (like Fourier series).

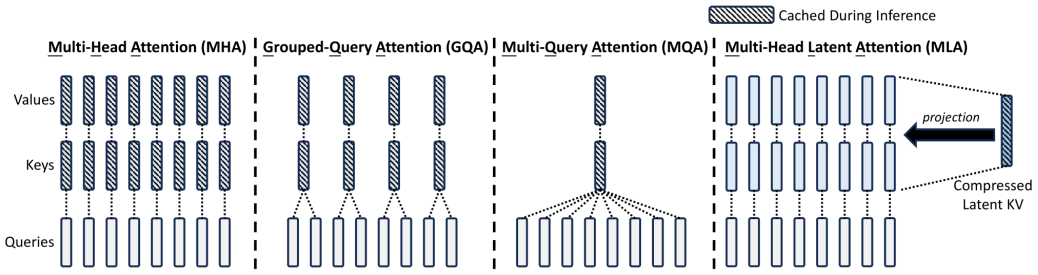
$$\mathbf{A}_{nk} = \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k \\ 0 & \text{else} \end{cases}$$

This matrix helps to compress the history of the information by masking the next tokens, which is similar to the masked self-attention. Note that the matrix just needs to be computed once.

Chapter 39

DeepSeek

39.1 Multi-Head Latent Attention



The query, key, and value of the vanilla multi-head attention can be expressed as follows:

$$\mathbf{q}_t = W^Q \mathbf{h}_t$$
$$\mathbf{k}_t = W^K \mathbf{h}_t$$
$$\mathbf{v}_t = W^V \mathbf{h}_t$$

- $\mathbf{q}_t, \mathbf{k}_t, \mathbf{v}_t \in \mathbb{R}^{d_h n_h}$
- $\mathbf{h}_t \in \mathbb{R}^d$: Attention input of the t-th token at an layer.
- d_h: the attention head's dimension
- n_h: the number of attention heads

During inference, all keys and values need to be cached to accelerate inference, so MHA needs to cache $2n_h d_h l$ elements (*i.e.,* key, value for each layer and head) for each token. In model deployment, this heavy KV cache is a large bottleneck that limits the maximum batch size and sequence length.

In DeepSeek The key idea of Multi-Head Latent Attention (MLA) is the low-rank joint compression

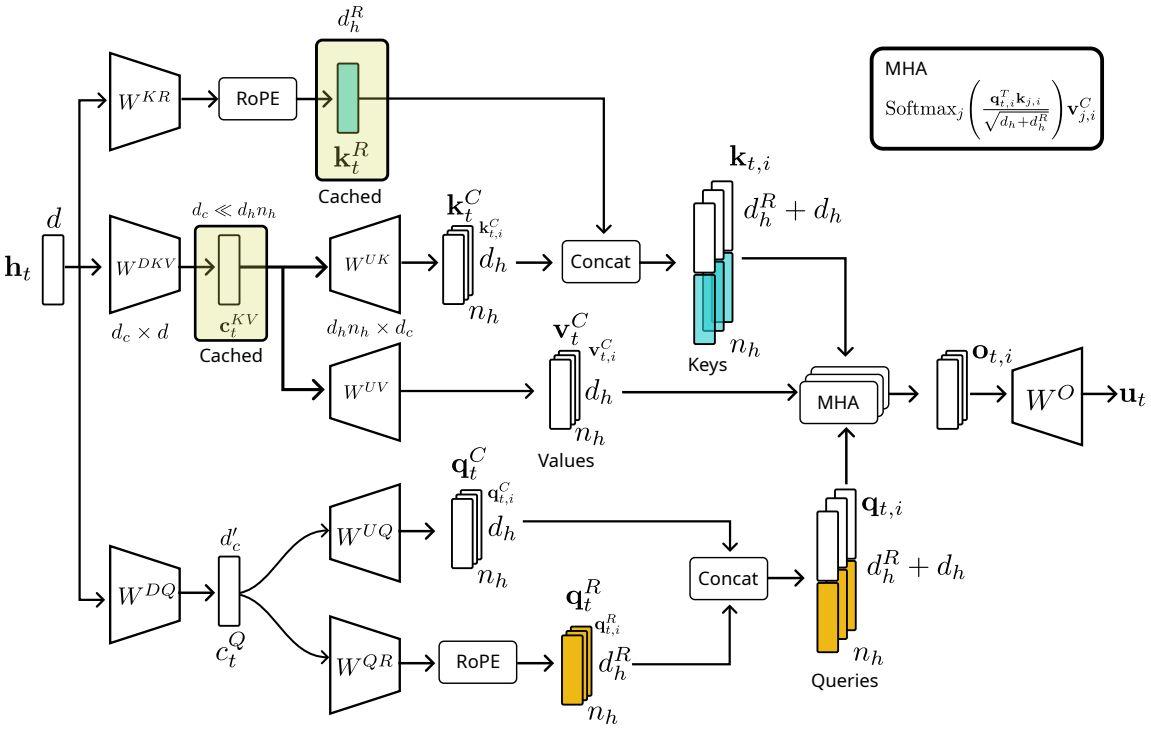


Figure 39.1: An overview of MLA.

for attention keys and values to reduce Key-Value (KV) cache during inference:

$$
\begin{aligned}
\mathbf{c}_t^{KV} &= W^{DKV}\mathbf{h}_t \\
[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C &= W^{UK}\mathbf{c}_t^{KV} \\
\mathbf{k}_t^R &= \text{RoPE}(W^{KR}\mathbf{h}_t) \\
\mathbf{k}_{t,i} &= [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R] \\
[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C &= W^{UV}\mathbf{c}_t^{KV}
\end{aligned}
$$

- D and U superscripts denote the up and down projection
- $\mathbf{c}_t^{KV} \in \mathbb{R}^{d_c}$ is the compressed (*i.e., c*) *latent vector* for keys and values, where $d_c \ll d_h n_h$. **Note that this is not a query vector.**
- $W^{DKV} \in \mathbb{R}^{d_c \times d}$ is the down-projection matrix
- $W^{UK}, W^{UV} \in \mathbb{R}^{d_h n_h \times d_c}$ are the up-projection matrices for keys and values, respectively.
- $W^{KR} \in \mathbb{R}^{d_h^R \times d}$ is the matrix used for generating the decoupled key of RoPE.
- **During inference, MLA only needs to cache $\mathbf{c}_t^{KV}$ and $\mathbf{k}_t^R$, which is a compressed latent vector, rather than high-dimensional key and value vector.** Thus, it can still have the multiple heads. This alleviates the issue of GQA or MQA while keeping their benefits.
- Also, we do not have to explicitly compute the key and the values for attention.

$$
\begin{aligned}
q_t^T k_t &= (W^{UQ} c_t^Q)^T (W^{UK} c_t^{KV}) \\
&= (c_t^Q)^T (W^{UQT} W^{UK}) c_t^{KV}
\end{aligned}
$$

– Here, $W^{UQT}W^{UK}$ is a combined matrix of the projection matrices.

Similarly, for values,

$$o_{t,i} = \text{AttnScore} \cdot v_t^C$$

The final output is

$$\begin{aligned} u_t &= W^O[o_{t,1}, \ldots, o_{t,n_h}] \\ &= W^O[\text{AttnScore} \cdot (W^{UV} c_t^{KV})] \\ &= W^O W^{UV}[\text{AttnScore} \cdot (c_t^{KV})] \end{aligned}$$

– To leverage this advantage, we need to use the *decoupled RoPE*. Otherwise, the RoPE would be coupled with projection matrices.

$$\mathbf{q}_t^T \mathbf{k}_t = (\mathbf{c}_t^Q)^T ((W^{UQ})^T W^{UK}) \mathbf{c}_T^{KV}$$

Moreover, in order to reduce the activation memory during training, we also perform low-rank compression for the queries, even if it cannot reduce the KV cache:

$$\begin{aligned} \mathbf{c}_t^Q &= W^{DQ}\mathbf{h}_t \\ [\mathbf{q}_{t,1}^C; \mathbf{q}_{t,2}^C; \ldots; \mathbf{q}_{t,n_h}^C] = \mathbf{q}_t^C &= W^{UQ}\mathbf{c}_t^Q \\ [\mathbf{q}_{t,1}^R; \mathbf{q}_{t,2}^R; \ldots; \mathbf{q}_{t,n_h}^R] = \mathbf{q}_t^R &= \text{RoPE}(W^{QR}\mathbf{c}_t^Q) \\ \mathbf{q}_{t,i} &= [\mathbf{q}_{t,i}^C; \mathbf{q}_{t,i}^R] \end{aligned}$$

- $\mathbf{c}_t^Q \in \mathbb{R}^{d'_c}$ is the compressed latent vector for queries, where $d'_c \ll d_h n_h$
- $W^{DQ} \in \mathbb{R}^{d'_c \times d}$ and $W^{UQ} \in \mathbb{R}^{d_h n_h \times d'_c}$ are the down- and up- projection matrices for queries, respectively.
- $W^{QR} \in \mathbb{R}^{d_h^R n_h \times d'_c}$ is the matrix for decoupled queries of RoPE.

Finally, the attention queries ($\mathbf{q}_{t,i}$), keys ($\mathbf{k}_{j,i}$), and values ($\mathbf{v}_{j,i}^C$) are combined to yield the final attention output $\mathbf{u}_t$:

$$\begin{aligned} \mathbf{o}_{t,i} &= \sum_{j=1}^{t} \text{Softmax}_j \left(\frac{\mathbf{q}_{t,i}^T \mathbf{k}_{j,i}}{\sqrt{d_h + d_h^R}} \right) \mathbf{v}_{j,i}^C, \\ \mathbf{u}_t &= W^O[\mathbf{o}_{t,1}; \mathbf{o}_{t,2}; \ldots; \mathbf{o}_{t,n_h}], \end{aligned}$$

where $W^O \in \mathbb{R}^{d \times d_h n_h}$ is the output projection matrix.

39.2 DeepSeek MoE

This paper mentioned that the conventional TopK MoE has Knowledge Hybridity and Knowledge Redundancy. Knowledge Hybridity: existing MoE practices often employ a limited number of experts (e.g., 8 or 16), and thus tokens assigned to a specific expert will be likely to cover diverse knowledge. Consequently, the designated expert will intend to assemble vastly different

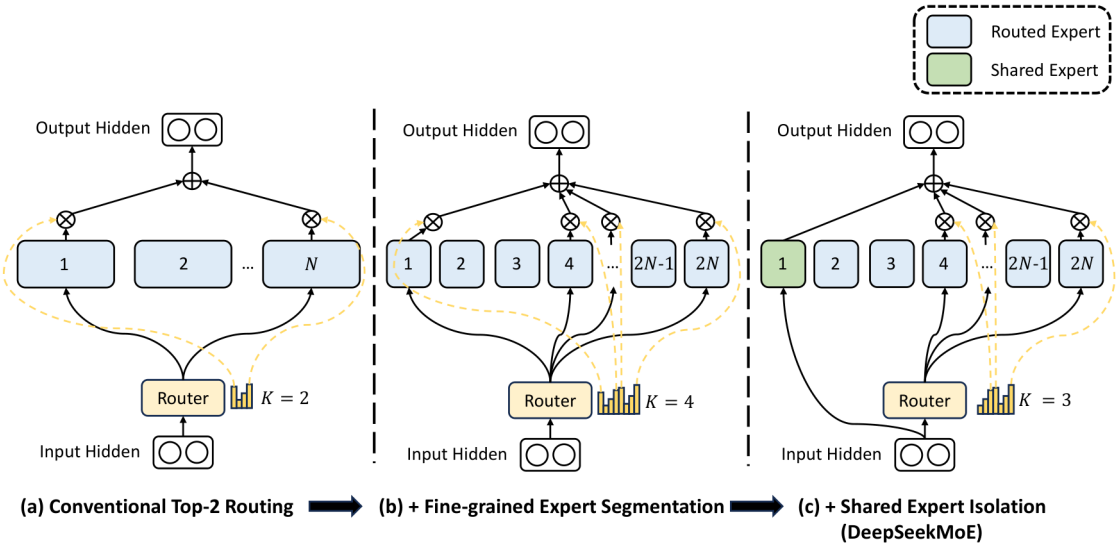


Figure 39.2: An overview of DeepSeek MoE.

types of knowledge in its parameters, which are hard to utilize simultaneously. (2) Knowledge Redundancy: tokens assigned to different experts may require common knowledge. As a result, multiple experts may converge in acquiring shared knowledge in their respective parameters, thereby leading to redundancy in expert parameters. These issues collectively hinder the expert specialization in existing MoE practices, preventing them from reaching the theoretical upper-bound performance of MoE models. By finely segmenting to more experts and introducing shared experts, DeepSeekMoE mitigated above two issues.

A typical practice to construct an MoE language model usually substitutes FFNs in a Transformer with MoE layers at specified intervals. An MoE layer is composed of multiple experts, where each expert is structurally identical to a standard FFN. Then, each token will be assigned to one or two experts. If the -th FFN is substituted with an MoE layer, the computation for its output hidden state h is expressed as:

$$\mathbf{h}'_t = \mathbf{u}_t + \sum_{i=1}^{N_s} FFN_i^{(s)}(\mathbf{u}_t) + \sum_{i=1}^{N_r} g_{i,t} FFN_i^{(r)}(\mathbf{u}_t),$$

- $$g_{i,t} = \frac{g'_{i,t}}{\sum_{j=1}^{N_r} g'_{j,t}},$$

  where

$$g'_{i,t} = \begin{cases} s_{i,t} & s_{i,t} \in TopK(\{s_{j,t} | 1 \le j \le N_r\}, K_r) \\ 0 & \text{otherwise,} \end{cases}$$

$$s_{i,t} = \sigma(\mathbf{u}_t^T \mathbf{e}_i)$$

- $\mathbf{u}_t$: FFN input of the t-th token.
- $\mathbf{h}'_t$ FFN output
- N_s and N_r are the number of *shared* experts and the *routed* experts, respectively.

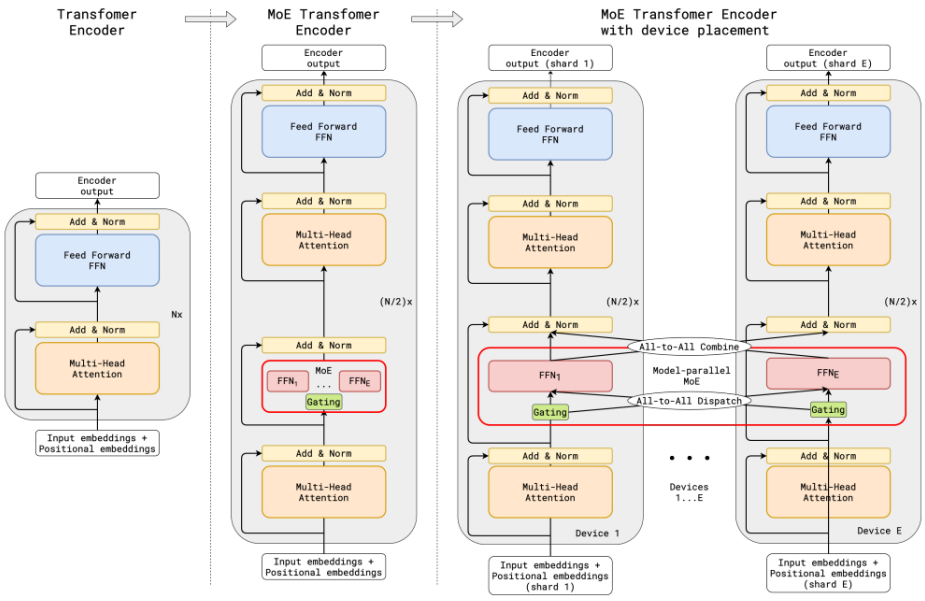


Figure 39.3: MoE Transformer Encoder from the GShard Paper

- $FFN_i^{(s)}(\cdot)$ and $FFN_i^{(r)}(\cdot)$ are the i-th *shared* expert and the i-th *routed* expert, respectively.
  - The shared experts are always activated, aiming at capturing and consolidating common knowledge across varying contexts.
  - Through compressing common knowledge into these shared experts, redundancy among other routed experts will be mitigated.
- K_r is the number of activated routed experts
- $g_{i,t}$: gating value for the i-th expert, which is sparse by its nature.
- $s_{i,t}$: a token assigned to an expert (*i.e.,* affinity score)
- $\mathbf{e}_i$: the centroid vector of the i-th (routed) expert
  - This is an (learnable) expert embedding representing assignment scores for each token claimed by each expert. The shared expert would get a vector like $\mathbf{1}$, which is a vector of ones.
- $TopK(\cdot, K)$: the set comprising K highest scores among the affinity scores calculated for the t-th token and all routed experts.
- σ: Sigmoid function.

Let's closely look at the equation

$$\mathbf{h}'_t = \mathbf{u}_t + \sum_{i=1}^{N_s} FFN_i^{(s)}(\mathbf{u}_t) + \sum_{i=1}^{N_r} g_{i,t} FFN_i^{(r)}(\mathbf{u}_t),$$

- $\mathbf{u}_t + \ldots$: this is just a skip connection
- $\sum_{i=1}^{N_s} FFN_i^{(s)}(\mathbf{u}_t)$: Always activated

- $\sum_{i=1}^{N_r} g_{i,t} FFN_i^{(r)}(\mathbf{u}_t)$
  - Here, we can notice that $g_{i,t}$ is the weight for the corresponding (routed) experts

To balance the load of the experts, DeepSeek also introduces a bias term b_i for each expert and add it to the corresponding scores $s_{i,t}$ as follows:

$$g'_{i,t} = \begin{cases} s_{i,t} & s_{i,t} + b_i \in TopK(\{s_{j,t} + b_i | 1 \leq j \leq N_r\}, K_r) \\ 0 & \text{otherwise,} \end{cases}$$

During training, the bias term decreases by γ at the end of each step if its corresponding expert is overloaded.

39.3 Multi-Token Prediction

DeepSeek also adopts a multi-token prediction approach and they show that it can improve the output quality and generalization behaviors. One of potential reasons would be that MTP may mitigate the distributional discrepancy between training time teacher forcing and inference time autoregressive generation.

Unlike the conventional MTP approach, they keep the complete causal chain at each prediction depth by introducing MTP modules.

The input tokens $[t_1, t_2, t_3, t_4]$ go through the main model's transformer blocks and then go through the output head of main model to produce next predicted token t_5. Meanwhile the representation of the input tokens $[t_1, t_2, t_3, t_4]$ (*i.e.,* output of main model's transformer blocks) will be passed to the MTP module and combine them with new input tokens' embedding$[t_2, t_3, t_4, t_5]$ to help produce additional token t_6. In DeepSeek-V3, the model is designed to predict next 2 tokens.

$$\mathbf{h}_i^{'k} = M_k[\text{RMSNorm}(\mathbf{h}_i^{k-1}); \text{RMSNorm}(\text{Emb}(t_{i+k}))]$$

- $\mathbf{h}_i^{k-1}$: i-th token at the $(k-1)$-th depth
- $(i+k)$-th token embedding $\text{Emb}(t_{i+k})$

39.4 Reinforcement Learning

39.4.1 Backgrounds: Proximal Policy Optimization

The objective function of Proximal Policy Optimization (PPO) can be represented as follows:

$$\theta_{k+1} = \underset{\theta}{\text{argmax}} \underset{s,a \sim \pi_{\theta_k}}{\mathbb{E}} [L(s, a, \theta_k, \theta)],$$

where θ_k is a parameter of a policy network at k-th step, θ is the current policy we want to update, and the A is the advantage (*i.e.,* reward). Finally, the L is given by

$$L(s, a, \theta_k, \theta) = \min \left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A^{\pi_{\theta_k}}(s, a),\ \text{Clip}\left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)}, 1-\varepsilon, 1+\varepsilon \right) A^{\pi_{\theta_k}}(s, a) \right).$$

Roughly, ε is a hyperparameter which says how far away the new policy is allowed to go from the old one. A simpler expression of the above expression is

$$L(s,a,\theta_k,\theta) = \min\left(\frac{\pi_\theta\left(a|s\right)}{\pi_{\theta_\mathrm{k}}\left(a|s\right)}A^{\pi_{\theta_k}}(s,a), g(\varepsilon, A^{\pi_{\theta_k}}(s,a))\right), \tag{39.1}$$

where

$$g(\varepsilon, A) = \begin{cases}(1+\varepsilon)A & A \geq 0\\ (1-\varepsilon)A & A < 0.\end{cases} \tag{39.2}$$

1. Positive Advantage: Suppose the advantage for that state-action pair is positive, in which case its contribution to the objective reduces to

$$L(s,a,\theta_k,\theta) = \min\left(\frac{\pi_\theta\left(a|s\right)}{\pi_{\theta_\mathrm{k}}\left(a|s\right)}, 1+\varepsilon\right)A^{\pi_{\theta_k}}(s,a). \tag{39.3}$$

   As the advantage is positive, the objective will increase if the action becomes more likely that is, if $\pi_\theta(a|s)$ increases. But the min in this term puts a limit to how much the objective can increase. Once $\pi_\theta(a|s) > (1+\epsilon)\pi_{\theta_k}(a|s)$, the min kicks in and this term hits a ceiling of $(1+\epsilon)A^{\pi_{\theta_k}}(s,a)$. Thus, the new policy does not benefit by going far away from the old policy.

2. Negative Advantage: Suppose the advantage for that state-action pair is negative, in which case its contribution to the objective reduces to

$$L(s,a,\theta_k,\theta) = \max\left(\frac{\pi_\theta\left(a|s\right)}{\pi_{\theta_\mathrm{k}}\left(a|s\right)}, 1-\varepsilon\right)A^{\pi_{\theta_k}}(s,a). \tag{39.4}$$

   Since the advantage is negative, the objective will increase if the action becomes less likely. In other words, if $\pi_\theta(a|s)$ decreases. But the max in this term puts a limit to how much the objective can increase. Once $\pi_\theta(a|s) < (1-\epsilon)\pi_{\theta_k}(a|s)$, the max kicks in and this term hits a ceiling of $(1-\epsilon)A^{\pi_{\theta_k}}(s,a)$. Thus, again, the new policy does not benefit by going far away from the old policy.

In sum, **clipping serves as a regularizer** by restricting the rewards to the policy, which change it dramatically with the hyperparameter ϵ corresponds to how far away the new policy can go from the old while still profiting the objective.

39.4.2 Group Relative Policy Optimization

Similarly, in DeepSeek, they leveraged a RL objective called Group Relative Policy Optimization (GRPO), which is a variant of PPO.

$$\mathcal{J} = \frac{1}{G}\sum_{i=1}^{G}\min\left(\frac{\pi_\theta\left(o_i|q\right)}{\pi_{\theta_\mathrm{k}}\left(o_i|q\right)}A_i,\ \mathrm{Clip}\left(\frac{\pi_\theta\left(o_i|q\right)}{\pi_{\theta_\mathrm{k}}\left(o_i|q\right)}, 1-\varepsilon, 1+\varepsilon\right)A_i\right) - \beta D_{KL}(\pi_\theta\|\pi_{\mathrm{ref}}).$$

- GRPO samples a group of outputs $\{o_1, o_2, \ldots, o_G\}$ from the old policy π_{θ_k} and then optimizes the policy model by maximizing the objective

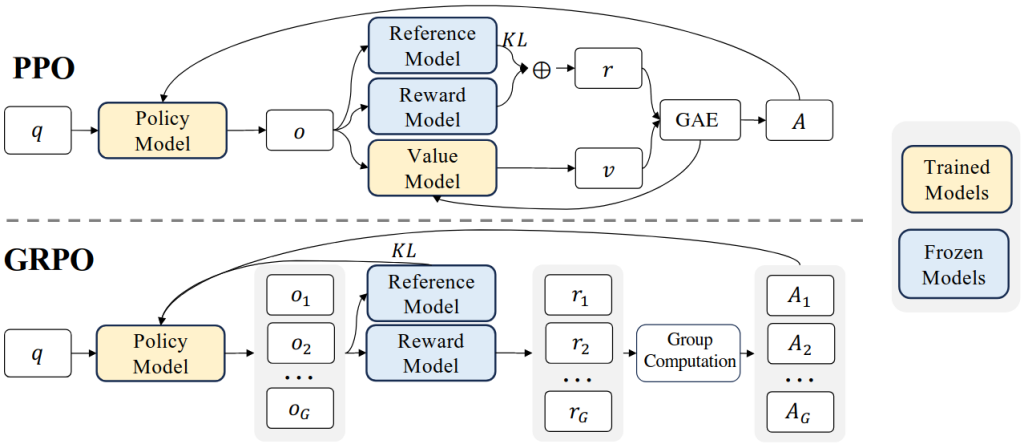


Figure 39.4: An illustration of GRPO. The policy model π takes an question (*i.e.,* observation, q) and generates answers (*i.e.,* actions, o_1) of the question.

- The KL-divergence is used to restrict the sudden change of policy.
- The advantage can be calculated by averaging and normalizing the rewards.
- Instead of using a value model explicitly, GRPO computes a value of the states (*i.e.,* o_i) by averaging them.
  - $A(s,a) = Q(s,a) - V(s)$
- π_{ref} is the reference model, which is an initial SFT model.

39.5 DeepSeek-R1

- DeepSeek-R1-Zero, which applies RL directly to the base model without any SFT data,
- DeepSeek-R1, which applies RL starting from a checkpoint fine-tuned with thousands of long Chain-of-Thought (CoT) examples.
- Distill the reasoning capability from DeepSeek-R1 to small dense models.

39.5.1 DeepSeek-R1-Zero

The reward is the source of the training signal, which decides the optimization direction of RL. To train DeepSeek-R1-Zero, we adopt a rule-based reward system that mainly consists of two types of rewards:

- Accuracy rewards: The accuracy reward model evaluates whether the response is correct. For example, in the case of math problems with deterministic results, the model is required to provide the final answer in a specified format (*e.g.,* within a box), enabling reliable rule-based verification of correctness. Similarly, for LeetCode problems, a compiler can be used to generate feedback based on predefined test cases.

Question: If $a > 1$, then the sum of the real solutions of $\sqrt{a - \sqrt{a + x}} = x$ is equal to
Response: <think> To solve the equation $\sqrt{a - \sqrt{a + x}} = x$, let's start by squaring both $\cdots$ $\left(\sqrt{a - \sqrt{a + x}}\right)^2 = x^2 \implies a - \sqrt{a + x} = x^2$. Rearrange to isolate the inner square root term: $(a - x^2)^2 = a + x \implies a^2 - 2ax^2 + (x^2)^2 = a + x \implies x^4 - 2ax^2 - x + (a^2 - a) = 0$ $\ldots$ Wait, wait. Wait. That's an aha moment I can flag here. Let's reevaluate this step-by-step to identify if the correct sum can be $\cdots$ We started with the equation: $\sqrt{a - \sqrt{a + x}} = x$ First, let's square both sides: $a - \sqrt{a + x} = x^2 \implies \sqrt{a + x} = a - x^2$ Next, I could square both sides again, treating the equation: $\cdots$ $\ldots$

- Format rewards: In addition to the accuracy reward model, we employ a format reward model that enforces the model to put its thinking process between <think> and </think> tags.

Note that *R1 does not use a neural reward model.*

Aha Moment of DeepSeek-R1-Zero A particularly intriguing phenomenon observed during the training of DeepSeek-R1-Zero is the occurrence of an aha moment. This moment, as illustrated in Table 3, occurs in an intermediate version of the model. During this phase, **DeepSeek-R1-Zero learns to allocate more thinking time to a problem by reevaluating its initial approach.** This behavior is not only a testament to the model's growing reasoning abilities but also a captivating example of how reinforcement learning can lead to unexpected and sophisticated outcomes.

This moment is not only an aha moment for the model but also for the researchers observing its behavior. It underscores the power and beauty of reinforcement learning: rather than explicitly teaching the model on how to solve a problem, we simply provide it with the right incentives, and it autonomously develops advanced problem-solving strategies. The aha moment serves as a powerful reminder of the potential of RL to unlock new levels of intelligence in artificial systems, paving the way for more autonomous and adaptive models in the future.

39.5.2 DeepSeek-R1

We construct and collect a small amount of long CoT data (thousands) to fine-tune the model as the initial RL actor.

- A key limitation of DeepSeek-R1-Zero is that its content is often not suitable for reading
- In contrast, when creating cold-start data for DeepSeek-R1, we design a readable pattern that includes a summary at the end of each response and filters out responses that are not reader-friendly. Here, we define the output format as |special-token|<reasoning-process>|special-token|<summary>, where the reasoning process is the CoT for the query, and the summary is used to summarize the reasoning results.

When reasoning-oriented RL converges, we utilize the resulting checkpoint to collect SFT (Supervised Fine-Tuning) data for the subsequent round. Unlike the initial cold-start data, which

primarily focuses on reasoning, this stage incorporates data from other domains to enhance the model's capabilities in writing, role-playing, and other general-purpose tasks. Specifically, we generate the data and fine-tune the model as described below.

We curate reasoning prompts and generate reasoning trajectories by performing rejection sampling from the checkpoint from the above RL training. In the previous stage, we only included data that could be evaluated using rule-based rewards. However, in this stage, we expand the dataset by incorporating additional data, some of which use a generative reward model by feeding the ground-truth and model predictions into DeepSeek-V3 for judgment. Additionally, because the model output is sometimes chaotic and difficult to read, we have filtered out chain-of-thought with mixed languages, long parapraphs, and code blocks. For each prompt, we sample multiple responses and retain only the correct ones. In total, we collect about 600k reasoning related training samples.

To equip more efficient smaller models with reasoning capabilities like DeepSeek-R1, we directly fine-tuned open-source models like Qwen (Qwen, 2024b) and Llama (AI@Meta, 2024) using the 800k samples curated with DeepSeek-R1.

Part VII

Appendix

Chapter 40

Vector Calculus

1.1 Differentiate

1.1.1 Differentiation Rules

- Product rule:
$$(f(x)g(x))' = f'(x)g(x) + f(x)g'(x)$$
- Quotient rule:
$$\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) + f(x)g'(x)}{(g(x))^2}$$
- Sum rule:
$$(f(x) + g(x))' = f'(x) + g'(x)$$
- Chain rule:
$$(g(f(x)))' = g'(f(x))f'(x)$$

The generalization of the derivative to functions of several variables is the *gradient*. We find the gradient of the function f with respect to x by varying one variable at a time and keeping the others constant. **The gradient is then the collection of these partial derivatives**.

For example, partial derivatives using the chain rule of $f(x, y) = (x + 2y^3)^2$ is given by
$$\frac{\partial f(x,y)}{\partial x} = 2(x + 2y^3)\frac{\partial}{\partial x}(x + 2y^3) = 2(x + 2y^3)$$

Basic rules of Partial Differentiation:

- Product rule:
$$\frac{\partial}{\partial \mathbf{x}}\big[f(\mathbf{x})g(\mathbf{x})\big] = \frac{\partial f}{\partial \mathbf{x}}g(\mathbf{x}) + f(\mathbf{x})\frac{\partial g}{\partial \mathbf{x}}$$
- Sum rule:
$$\frac{\partial}{\partial \mathbf{x}}\big[f(\mathbf{x}) + g(\mathbf{x})\big] = \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial g}{\partial \mathbf{x}}$$
- Chain rule:
$$\frac{\partial}{\partial \mathbf{x}}(g \circ f)(\mathbf{x}) = \frac{\partial}{\partial \mathbf{x}}\big[g(f(\mathbf{x}))\big] = \frac{\partial g}{\partial f}\frac{\partial f}{\partial \mathbf{x}}$$

2.2 Chain Rule

Consider a function $f : \mathbb{R}^2 \to \mathbb{R}$ of two variables x_1 and x_2. They are functions of t, $x_1(t)$ and $x_2(t)$. To compute the gradient of f with respect to t, we need to apply the chain rule for multivariate functions as

$$\frac{\partial f}{\partial t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1}\frac{\partial x_1(t)}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2(t)}{\partial t}$$

Given that $f(x_1, x_2)$ is a function of x_1 and x_2, where $x_1 = x_1(s,t)$ and $x_2 = x_2(s,t)$ are themselves functions of two variables s and t, the chain rule can be used to find the partial derivatives of f with respect to s and t.

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s}$$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t}$$

The gradient of f is obtained by the matrix multiplication as follows:

$$\frac{df}{d(s,t)} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial (s,t)} = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial s} & \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial s} & \frac{\partial x_2}{\partial t} \end{pmatrix}$$

3.3 Vector Notations

- $\mathbf{x} = (x_1, x_2, ..., x_n)$ or
- $$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

Differentiate a vector y by a scalar $\mathbf{x}$:

$$\frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \vdots \\ \frac{\partial y_n}{\partial x} \end{bmatrix}$$

Differentiate a scalar y by a vector $\mathbf{x}$:

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1}, \cdots, \frac{\partial y}{\partial x_n} \end{bmatrix}$$

Differentiate a vector y by a vector $\mathbf{x}$:

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_n} \end{bmatrix}$$

$\mathbf{a}^T\mathbf{x}$ is a scalar value, so

$$\begin{aligned} \frac{\partial \mathbf{a}^T\mathbf{x}}{\partial \mathbf{x}} &= \left[\frac{\partial(\mathbf{a}^T\mathbf{x})}{\partial x_1} \cdots \frac{\partial(\mathbf{a}^T\mathbf{x})}{\partial x_n} \right] = \left[\frac{\partial(a_1x_1 + \cdots + a_nx_n)}{\partial x_1}, \cdots, \frac{\partial(a_1x_1 + \cdots + a_nx_n)}{\partial x_n} \right] \\ &= [a_1, \ldots, a_n] = \mathbf{a}^T \end{aligned}$$

$$A\mathbf{x} = \begin{bmatrix} a_{11} & \ldots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \ldots & a_{mn} \end{bmatrix} \times \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n a_{1i}x_i \\ \vdots \\ \sum_{i=1}^n a_{mi}x_i \end{bmatrix}$$

Thus,

$$\frac{\partial A\mathbf{x}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial \sum_{i=1}^n a_{1i}x_i}{\partial x_1} & \cdots & \frac{\partial \sum_{i=1}^n a_{1i}x_i}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial \sum_{i=1}^n a_{mi}x_i}{\partial x_1} & \cdots & \frac{\partial \sum_{i=1}^n a_{mi}x_i}{\partial x_n} \end{bmatrix} = A$$

Chapter 41

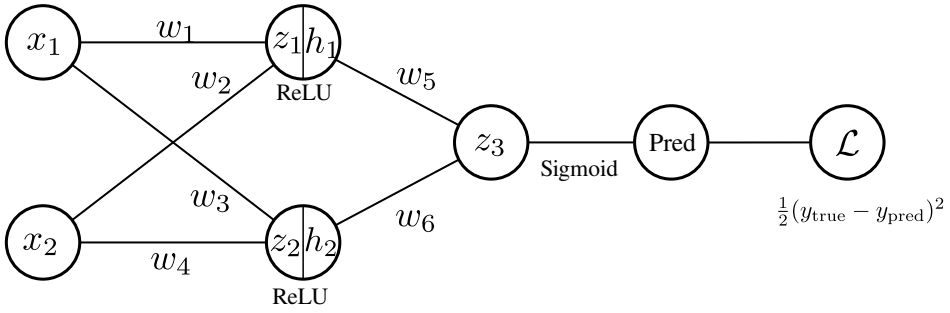
Backpropagation

1.1 Introduction

An area where the chain rule is used extensively is deep learning, where the function value y is computed as a many-level function composition:

$$y = (f_K \circ f_{K-1} \circ \cdots \circ f_1)(x) = f_K(f_{K-1}(\cdots(f_1(x))\cdots)),$$

where x are the inputs (e.g., images), y are the observations (e.g., class labels), and every function f_i, $i = 1, \ldots, K$, possesses its own parameters.



We have:

- Inputs: x_1, x_2.
- Hidden layer: 2 neurons, each with no bias (for simplicity).
- Weights $w_1, w_2, w_3, w_4, w_5, w_6$
- Output layer: 1 neuron, also with no bias.

Where:

- $z_1 = w_1\, x_1 + w_2\, x_2, \quad h_1 = \text{ReLU}(z_1)$
- $z_2 = w_3\, x_1 + w_4\, x_2, \quad h_2 = \text{ReLU}(z_2)$
- $z_3 = w_5\, h_1 + w_6\, h_2, \quad y_{\text{pred}} = \sigma(z_3)$

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

We will train on one example $\{x = [x_1, x_2], y_{\text{true}}\}$.

Loss function: Mean Squared Error (MSE) for one sample:

$$L = \frac{1}{2} \left(y_{\text{pred}} - y_{\text{true}}\right)^2.$$

We want to find the partial derivatives:

$$\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, \frac{\partial L}{\partial w_3}, \frac{\partial L}{\partial w_4}, \frac{\partial L}{\partial w_5}, \frac{\partial L}{\partial w_6}.$$

Useful Derivatives:

- Derivative of the MSE loss (single sample):

$$\frac{\partial L}{\partial y_{\text{pred}}} = \left(y_{\text{pred}} - y_{\text{true}}\right).$$

- Sigmoid derivative:

$$\frac{d}{dz}\,\sigma(z) = \sigma(z)\left(1 - \sigma(z)\right).$$

  So,

$$\frac{\partial y_{\text{pred}}}{\partial z_3} = y_{\text{pred}}\,(1 - y_{\text{pred}}).$$

- Chain rule:

$$\frac{\partial L}{\partial z_3} = \frac{\partial L}{\partial y_{\text{pred}}} \times \frac{\partial y_{\text{pred}}}{\partial z_3}.$$

The output node has:

$$z_3 = w_5\, h_1 + w_6\, h_2, \quad y_{\text{pred}} = \sigma(z_3).$$

First, find $\frac{\partial L}{\partial z_3}$:

$$\frac{\partial L}{\partial z_3} = (y_{\text{pred}} - y_{\text{true}}) \times \left[y_{\text{pred}}\,(1 - y_{\text{pred}})\right].$$

Then,

$$\frac{\partial L}{\partial w_5} = \frac{\partial L}{\partial z_3} \times \frac{\partial z_3}{\partial w_5} = \frac{\partial L}{\partial z_3} \times h_1.$$

Since $z_3 = w_5\, h_1 + w_6\, h_2$, so $\partial z_3 / \partial w_5 = h_1$.

Each hidden neuron influences the output via h_1 or h_2. Let's do them one neuron at a time.

4.3.1. Hidden Neuron1 (w_1, w_2)

$$z_1 = w_1\, x_1 + w_2\, x_2, \quad h_1 = \sigma(z_1).$$

To get $\frac{\partial L}{\partial w_1}$, we chain through:

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial z_3} \times \frac{\partial z_3}{\partial h_1} \times \frac{\partial h_1}{\partial z_1} \times \frac{\partial z_1}{\partial w_1}.$$

- We already have $\frac{\partial L}{\partial z_3} = -0.12058$. - $\frac{\partial z_3}{\partial h_1} = w_5$ (since $z_3 = w_5\, h_1 + w_6\, h_2$). - $\frac{\partial h_1}{\partial z_1} = \sigma(z_1)\big(1 - \sigma(z_1)\big) = h_1\,(1 - h_1)$. - $\frac{\partial z_1}{\partial w_1} = x_1$.

Numerically:

1. $\frac{\partial z_3}{\partial h_1} = w_5 = 0.2$. 2. $h_1(1 - h_1) = 0.62246 \times (1 - 0.62246) = 0.62246 \times 0.37754 \approx 0.2350$. 3. $x_1 = 1.0$.

So,

$$\frac{\partial L}{\partial w_1} = (-0.12058) \times (0.2) \times (0.2350) \times (1.0).$$

Compute step by step:

- $(-0.12058) \times 0.2 = -0.024116$. - $(-0.024116) \times 0.2350 \approx -0.005667$.

Thus,

$$\frac{\partial L}{\partial w_1} \approx -0.005667.$$

For w_2, the only difference is $\frac{\partial z_1}{\partial w_2} = x_2$. Since $x_2 = 0.0$ in our example, it follows immediately:

$$\frac{\partial L}{\partial w_2} = 0.$$

4.3.2. Hidden Neuron2 (w_3, w_4)

$$z_2 = w_3\, x_1 + w_4\, x_2, \quad h_2 = \sigma(z_2).$$

By the same chain rule:

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial z_3} \times \frac{\partial z_3}{\partial h_2} \times \frac{\partial h_2}{\partial z_2} \times \frac{\partial z_2}{\partial w_3}.$$

- We have $\frac{\partial L}{\partial z_3} = -0.12058$. - $\frac{\partial z_3}{\partial h_2} = w_6 = -0.1$. - $\frac{\partial h_2}{\partial z_2} = h_2(1 - h_2) = 0.57444 \times 0.42556 \approx 0.24450$. - $\frac{\partial z_2}{\partial w_3} = x_1 = 1.0$.

So,

$$\frac{\partial L}{\partial w_3} = (-0.12058) \times (-0.1) \times (0.24450) \times (1.0).$$

Compute step by step:

1. $(-0.12058) \times (-0.1) = 0.012058$. 2. $0.012058 \times 0.24450 \approx 0.002950$.

Hence,

$$\frac{\partial L}{\partial w_3} \approx 0.002950.$$

For w_4, again $\partial z_2/\partial w_4 = x_2 = 0$, so:

$$\frac{\partial L}{\partial w_4} = 0.$$

—

5. Weight Update

Let's do **one step** of Gradient Descent with learning rate $\eta = 0.1$. The update rule is:

$$w_i \leftarrow w_i - \eta \frac{\partial L}{\partial w_i}.$$

5.1. Final Gradients Recap

- $\frac{\partial L}{\partial w_1} \approx -0.005667$ - $\frac{\partial L}{\partial w_2} = 0$ - $\frac{\partial L}{\partial w_3} \approx 0.002950$ - $\frac{\partial L}{\partial w_4} = 0$ - $\frac{\partial L}{\partial w_5} \approx -0.07509$ - $\frac{\partial L}{\partial w_6} \approx -0.06930$

5.2. Updated Weights

1. w_1:
$$w_1 \leftarrow 0.5 - 0.1 \times (-0.005667) = 0.5 + 0.0005667 \approx 0.50057.$$

2. w_2:
$$w_2 \leftarrow -0.5 - 0.1 \times 0 = -0.5.$$

3. w_3:
$$w_3 \leftarrow 0.3 - 0.1 \times (0.002950) = 0.3 - 0.000295 \approx 0.299705.$$

4. w_4:
$$w_4 \leftarrow 0.1 - 0.1 \times 0 = 0.1.$$

5. w_5:
$$w_5 \leftarrow 0.2 - 0.1 \times (-0.07509) = 0.2 + 0.007509 \approx 0.20751.$$

6. w_6:
$$w_6 \leftarrow -0.1 - 0.1 \times (-0.06930) = -0.1 + 0.00693 \approx -0.09307.$$

—

Recap

1. **Forward pass**: - Calculated hidden neurons z_1, z_2, then h_1, h_2. - Calculated output z_3, then y_{pred}. - Computed the MSE loss L.

2. **Backward pass**: - Used the chain rule to find $\frac{\partial L}{\partial w_i}$ for each weight. - Observed how zero input ($x_2 = 0$) caused some gradients to be zero for this training example.

3. **Gradient Descent update**: - Applied $w_i \leftarrow w_i - \eta \, (\partial L / \partial w_i)$ with $\eta = 0.1$.

While we only did one training example and one update step, the principle is the same for multiple samples (you would sum or average the gradients across the batch). Larger networks just repeat the same chain-rule logic on more layers and neurons.

That's it! This is the backpropagation process laid out in a small, fully traceable network with two hidden neurons. By doing the arithmetic yourself, you can see exactly how each weight nudges the output and how the gradients flow backward to update those weights.

Chapter 42

Divergence

1.1 KL Divergence between Two Normal Distribution

$$D_{\mathrm{KL}}(P||Q) = \mathbb{E}_P\Big[\log\frac{P}{Q}\Big]$$

Consider two multivariate Gaussians in $\mathbb{R}^n$, P_1 and P_2

$$\begin{aligned}
D_{\mathrm{KL}}(P||Q) &= \int \left[\frac{1}{2}\log\frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2)\right] \times p(x)dx \\
&= \frac{1}{2}\log\frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2}\mathrm{tr}\left\{E[(x-\mu_1)(x-\mu_1)^T]\ \Sigma_1^{-1}\right\} + \frac{1}{2}E[(x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2)] \\
&= \frac{1}{2}\log\frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2}\mathrm{tr}\ \{I_n\} + \frac{1}{2}(\mu_1-\mu_2)^T\Sigma_2^{-1}(\mu_1-\mu_2) + \frac{1}{2}\mathrm{tr}\{\Sigma_2^{-1}\Sigma_1\} \\
&= \frac{1}{2}\left[\log\frac{|\Sigma_2|}{|\Sigma_1|} - n + \mathrm{tr}\{\Sigma_2^{-1}\Sigma_1\} + (\mu_2-\mu_1)^T\Sigma_2^{-1}(\mu_2-\mu_1)\right]
\end{aligned}$$

Trace tricks:

$$x^TAx = tr[x^TAx] = tr[xx^TA]$$
$$tr[A+B] = tr[A] + tr[B]$$
$$E[(x-\mu)^T\Sigma^{-1}(x-\mu)] = tr(E[(x-\mu)(x-\mu)^T]\Sigma^{-1})$$
$$\Sigma = E[(X-\mu)(X-\mu)^T] = E[XX^T] - \mu\mu^T$$
$$E[XX^T] = \Sigma + \mu\mu^T$$

Note that the determinant of a diagonal matrix could be computed as product of its diagonal.

2.2 Various Tricks

2.2.1 Spectral Normalization

A persisting challenge in the training of GANs is the performance control of the discriminator. The derivative of discriminator could be unbounded and even incomputable, so they introduced a regularization on the derivative of discriminator called, Lipchitz continuity, which bound the gradient.

Neural network is actually a composite function. So if we make each function to satisfy the Lipchitz continuity, then we can make whole network satisfy it. Lipchitz continuity of a linear operator can be seen as

$$
\begin{aligned}
||f(x_1) - f(x_2)||_2 &\leq L||x_1 - x_2||_2 \\
||Ax_1 - Ax_2||_2 &\leq L||x_1 - x_2||_2 \\
\frac{||Ax||_2}{||x||_2} &\leq L \\
\sigma_{max} \underbrace{\sup_x \frac{||Ax||_2}{||x||_2}}_{SpectralNorm} &\leq L, \quad \text{Since inequaility holds for all } x
\end{aligned}
$$

, where σ_{max} is the maximum singular value. Note that the spectral norm is from the linear algebra. We can make the matrix A Lipchitz continuous by

$$
1 = \underbrace{\sup_x \frac{||\frac{A}{\sigma_{max}}x||_2}{||x||_2}}_{SpectralNorm} \leq L
$$

2.2.2 Moving Averaging

2.2.3 Weight Averaging

2.2.4 Quality Measurements

3.3 f-Divergence

In probability theory, an f-divergence is a function $D_f(p||q)$ that measures the difference between two probability distributions p and q. It helps the intuition to think of the divergence as an average, weighted by the function f, of the odds ratio given by p and q.

For distributions p and q, f-divergence is defined as:

$$
D_f(p||q) = \int_{\mathcal{X}} f\left(\frac{p(x)}{q(x)}\right) q(x) dx
$$

- KL-divergence: $f(t) = t \log t$

- Reversed KL-divergence: $f(t) = -\log t$
- Total variation: $f(t) = \frac{1}{2}|t-1|$

$$D_f(p||q) = \int_{\mathcal{X}} |p(x) - q(x)|dx$$

4.4 Lipchitz Continuous

The function f in the new form of Wasserstein metric is demanded to satisfy $\|f\|_L \leq K$, meaning it should be K-Lipschitz continuous.

A real-valued function $f : \mathbb{R} \to \mathbb{R}$ is called K-Lipschitz continuous if there exists a real constant $K \geq 0$ such that, for all $x_1, x_2 \in \mathbb{R}$

$$|f(x_1) - f(x_2)| \leq K|x_1 - x_2|$$

5.5 Singular Value

All singular values can be calculated via the singular value decomposition (SVD)

$$A = U\Sigma V^T$$

, where U is the left singular vectors and V is the right singular vectors. However, if we just want the maximum singular value then we just need to find corresponding vectors

$$\sigma = uAv^T$$

Actually, there is a simpler way to find the maximum singular value e.g., power iteration.

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