Statistics

1.1 Basics

- $E(X) = \int x f(x)$ and $Var(X) = E((X \mu)^2)$.
- Sample mean: $\overline{X} = \frac{1}{n} \sum X_i$.
- Sample variance: $S^2 = \frac{1}{n-1} \sum (X_i \overline{X})^2$.
- Likelihood: Let X_i have joint pdf $f(\mathbf{x}; \theta)$. Given observed values x_i of X_i , the *likelihood* of θ is $L(\theta) = f(\mathbf{x}; \theta)$. The maximum likelihood estimate $\hat{\theta}(\mathbf{x})$ is the value of θ that maximizes $L(\theta)$.

1.2 Convergence of Random Variables

RVs X_n with cdf F_n .

• X_n converges in distribution to X (weakly) if

$$\lim F_n(x) = F(x)$$

for all x at which F is continuous.

• X_n converges in probability to X if for all $\epsilon > 0$,

$$\lim P(|X_n - X| > \epsilon) = 0.$$

• X_n converges almost surely to X (strongly) if

$$P\left(\lim X_n = X\right) = 1,$$

i.e., events for which X_n does not converge to X have probability 0.

1.3 Parameter Estimation

An estimator is any statistic $\hat{\theta} = \hat{\theta}(X)$ used to estimate θ .

1.3.1 Properties of estimators

Mean squared error

• $MSE(\hat{\theta}) = E\left[(\hat{\theta} - \theta)^2\right].$

Variance

• $\operatorname{Var}(\hat{\theta}) = \operatorname{E}\left[(\hat{\theta} - \operatorname{E}(\hat{\theta}))^2\right].$

Bias

• Bias($\hat{\theta}$) = E($\hat{\theta}$) – θ .

• Note that $MSE(\hat{\theta}) = Var(\hat{\theta}) + Bias(\hat{\theta})^2$.

• The unbiased estimator with the smallest variance is known as the *minimum-variance unbiased estimator* (MVUE).

Consistency

• An estimator T_n of θ is weakly consistent if T_n converges in probability to θ .

• T_n is strongly consistent if T_n converges almost surely to θ .

Asymptotic normality

• T_n is asymptotically normal if

$$\sqrt{n}(T_n - \theta) \xrightarrow{D} N(0, V).$$

• Recall: CLT says that sample mean \overline{X} is asymptotically normal.

Efficiency

• The observed information is

$$J(\theta) = -\frac{d^2l}{d\theta^2}$$

for scalar parameter θ or

$$J(\theta)_{ij} = -\frac{\partial^2 l}{\partial \theta_i \partial \theta_j}$$

for $\theta = (\theta_1, \dots, \theta_p)$.

• The larger $J(\hat{\theta})$ is, the more concentrated $l(\theta)$ is about $\hat{\theta}$.

• The expected or Fisher information is

$$I(\theta) = E\left(-\frac{d^2l}{d\theta^2}\right)$$

or

$$I(\theta)_{ij} = \mathrm{E}\left(-\frac{\partial^2 l}{\partial \theta_i \partial \theta_j}\right).$$

• Equivalently, define score to be gradient of $l(\theta)$, i.e.,

$$s(\theta) = \frac{\partial l}{\partial \theta}.$$

Then expected value of score at θ is 0, i.e., $E(s \mid \theta) = 0$. The Fisher information is defined to be the variance of the score $Var(s(\theta)) = E(s(\theta)s(\theta)^T)$.

• The Cramer-Rao bound says that for an unbiased estimator,

$$\operatorname{Var}(\hat{\theta}) \ge \frac{1}{I(\theta)}.$$

Generally, if $E(\hat{\theta}) = \psi(\theta)$, then

$$\operatorname{Var}(\hat{\theta}) \ge \frac{(\psi'(\theta))^2}{I(\theta)} = \frac{(1+b'(\theta))^2}{I(\theta)},$$

where b is the bias. In the unbiased multivariate case, the Cramer-Rao bound states that

$$cov(T(X)) \ge I(\theta)^{-1}$$
,

where $M \geq 0$ means that M is positive semidefinite, i.e., $\mathbf{x}^T M \mathbf{x} \geq 0$ for all \mathbf{x} .

ullet The efficiency of an unbiased estimator is

$$e(T) = \frac{1/I(\theta)}{\text{Var}(T)}.$$

By the Cramer-Rao bound, we know $e(T) \leq 1$. An estimator is *efficient* if e(T) = 1 for all θ , i.e., achieves Cramer-Rao bound for all θ . Thus, an efficient estimator is the MVUE (but not necessarily conversely).

Properties of MLEs

Let $\hat{\theta}$ be the MLE of θ . Then

- $\sqrt{n}(\hat{\theta} \theta) \xrightarrow{D} N(0, I(\theta)^{-1})$, so $\hat{\theta}$ is asymptotically unbiased and asymptotically efficient.
- $\hat{\theta} \stackrel{(}{\to} P)\theta$, i.e., $\hat{\theta}$ is consistent.
- Invariance property: the MLE of $g(\theta)$ is $g(\hat{\theta})$.

1.4 Hypothesis Testing

 X_i random sample from $f(x;\theta)$.

- Setup:
 - Null hypothesis $H_0: \theta \in \Theta_0$
 - Alternative hypothesis $H_1: \theta \in \Theta_1$
- Construct test statistic $t(\mathbf{X})$ such that large values of $t(\mathbf{X})$ cast doubt on H_0 .

- Let $t_{\text{obs}} = t(\mathbf{x})$.
- The *p-value* or *significance level* is

$$p = P(t(\mathbf{X}) \ge t_{\text{obs}} \mid H_0).$$

- Small p-value = observed values unlikely under H_0 .
- Can define critical region to be C such that we reject H_0 if and only if $\mathbf{x} \in C$.

1.4.1 Errors in hypothesis testing

Two types of error:

- Type I error: rejecting H_0 when H_0 is true
- Type II error: not rejecting H_0 when H_0 is false.

The *size* of a test is defined by

$$\alpha = P(\text{type I error})$$

= $P(\text{reject } H_0 \mid H_0 \text{ true}).$

The *power* of a test is $1 - \beta$, where

$$\beta = P(\text{type II error})$$

= $P(\text{don't reject } H_0 \mid H_1 \text{ true}).$

We want small size and high power.

For composite H_i , define the size

$$\alpha = \sup \theta \in \Theta_0 P(\text{reject } H_0 \mid \theta)$$

and the power function

$$w(\theta) = P(\text{reject } H_0 \mid \theta).$$

We want $w \approx 0$ for $\theta \in \Theta_0$ and $w \approx 1$ for $\theta \in \Theta_1$.

Student's t-test

Consider statistic

$$t = \frac{\overline{x} - \mu_0}{s / \sqrt{n}},$$

which has t-distribution with n-1 degrees of freedom. Recall that a t-distribution is given by

$$T = \frac{Z}{\sqrt{V/\nu}},$$

where Z is standard normal and V is χ^2 with ν degrees of freedom.

Noncentral t-distribution

- Noncentral distributions describe how a test statistic is distributed when the null hypothesis is false.
- Noncentral t-distribution is given by

$$T = \frac{Z + \mu}{\sqrt{V/\nu}},$$

where μ is the noncentrality parameter.

• Under the alternative hypothesis, we get noncentral t-distribution with n-1 degrees of freedom and noncentrality parameter

$$\delta = \frac{\mu - \mu_0}{\sigma / \sqrt{n}}.$$

This allows us to set the power as

Power =
$$P(\text{reject } H_0 \mid H_1)$$
.

Note that as n increases, power increases.

1.5 Bayesian Inference

- Unknown parameters are random variables.
- Probability model $f(\mathbf{x} \mid \theta)$ that is conditional on the value of θ .
- Prior density $\pi(\theta)$.
- After using observed data \mathbf{x} , get posterior density $\pi(\theta \mid \mathbf{x})$.
- We have

$$\pi(\theta \mid \mathbf{x}) \propto f(\mathbf{x} \mid \theta) \times \pi(\theta)$$

posterior \propto likelihood \times prior

1.5.1 Prediction

- X_{n+1} future observation and $\mathbf{x} = (x_1, \dots, x_n)$ observed data.
- Assume, conditional on θ , that X_{n+1} has density $f(x_{n+1} \mid \theta)$ independent of X_i, \ldots, X_n .
- The density of X_{n+1} given \mathbf{x} , called the *posterior predictive density*, is a conditional density denoted $f(x_{n+1} \mid \mathbf{x})$.
- Then

$$f(x_{n+1} \mid \mathbf{x}) = \int f(x_{n+1}, \theta \mid \mathbf{x}) d\theta$$
$$= \int f(x_{n+1} \mid \theta, \mathbf{x}) \pi(\theta \mid \mathbf{x}) d\theta$$
$$= \int f(x_{n+1} \mid \theta) \pi(\theta \mid \mathbf{x}) d\theta$$

1.5.2 Credible interval

- Bayesian alternative to confidence interval.
- A $100(1-\alpha)\%$ credible set for θ is $jc \subset \Theta$ such that

$$P(\theta \in C \mid \mathbf{x}) = \int_C \pi(\theta \mid \mathbf{x}) d\theta = 1 - \alpha.$$

1.5.3 Hypothesis testing and Bayes factors

Setup

- Prior probabilities $P(H_i)$ such that $P(H_0) + P(H_1) = 1$.
- A prior for θ_i under H_i , denoted $\pi(\theta_i \mid H_i)$.
- A model for data **x** under H_i , denoted $f(\mathbf{x} \mid \theta_i, H_i)$.

Bayes factor

• Prior odds of H_0 relative to H_1 is

$$\frac{P(H_0)}{P(H_1)}$$

• Posterior odds of H_0 relative to H_1 is

$$\frac{P(H_0 \mid \mathbf{x})}{P(H_1 \mid \mathbf{x})}.$$

• Using Bayes' Theorem, get

$$\frac{P(H_0 \mid \mathbf{x})}{P(H_1 \mid \mathbf{x})} = \frac{P(\mathbf{x} \mid H_0)}{P(\mathbf{x} \mid H_1)} \times \frac{P(H_0)}{P(H_1)}$$

posterior odds = Bayes factor \times prior odds

where the Bayes factor of H_0 relative to H_1 is

$$B_{01} = \frac{P(\mathbf{x} \mid H_0)}{P(\mathbf{x} \mid H_1)}.$$

• The quantity

$$P(\mathbf{x} \mid H_i) = \int_{\Theta_i} f(\mathbf{x} \mid \theta_i, H_i) \pi(\theta_i \mid H_i) d\theta$$

is called the marginal likelihood for H_i .

Linear Regression

• Observations

$$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} + \epsilon_i = x_i \cdot \beta + \epsilon_i$$

i.e., $y = X\beta + \epsilon$.

• Loss function

$$L(\beta) = \text{MSE}(\beta) = \frac{1}{n} ||y - X\beta||^2.$$

- Want $\hat{\beta}$ that minimizes $L(\beta)$:
 - Find $\hat{\beta}$ such that

$$\frac{\partial L}{\partial \beta} = 0.$$

- Project y onto Col(X).

Get $\hat{\beta} = (X^T X)^{-1} X^T y$. For simple linear regression, i.e. $y = \beta_0 + \beta_1 x + \epsilon$, we get

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x},$$

$$\hat{\beta}_1 = \frac{\text{cov}(x, y)}{\text{Var}(x)} = \frac{\sum (x_i - \overline{x})(y_i - \overline{y})}{\sum (x_i - \overline{x})^2}.$$

- Residual is $\hat{\epsilon} = y X\hat{\beta}$. The residual/explained/total sum of squares is:
 - RSS = $\|\hat{e}\|^2$, i.e., variation in the error between the observed data and modeled values.
 - ESS = $\sum (\hat{y}_i \overline{y}_i)$, i.e., how much variation there is in the modeled values.
 - TSS = $\sum (y_i \overline{y})$, i.e., how much variation there is in the observed data.
 - In linear regression, TSS = RSS + ESS.
- Coefficient of determination is

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}.$$

Note that the baseline model always predicts \overline{y} , so $R^2 = 0$. Furthermore, adding features weakly decreases RSS, hence weakly increases R^2 . Instead, we could use adjusted R^2 :

$$\overline{R}^2 = 1 - \frac{\mathrm{RSS}/\mathrm{df_{res}}}{\mathrm{TSS}/\mathrm{df_{tot}}},$$

where df is degrees of freedom, so $df_{res} = n - p - 1$ and $df_{tot} = n - 1$.

• Assumptions:

- Weak exogeneity: Predictor variables x can be treated as fixed values, and not random variables, i.e., x is error-free, i.e., $E(x\epsilon) = 0$. So no confounding variables.
- **Linearity**: Mean of y is linear combination of parameters and x.
- **Independence**: Observations are independent of each other.
- **Homoscedasticity**: Constant variance of ϵ .
- Normality: ϵ follow a normal distribution.
- No multicollinearity: The independent variables are not highly correlated with each other.

Natural Language Processing

- Solve sequence transduction, i.e., transforms an input sequence to an output sequence.
- Necessary to have some *memory*.

3.1 RNN

- At each time step, receive two inputs: word embedding of current word and hidden state.
- Let $x_t \in \mathbb{R}^n$ and $h_{t-1} \in \mathbb{R}^m$.
- Use weight matrix $W_x \in \mathbb{R}^{m \times n}$ and hidden-state-to-hidden-state matrix $W_h \in \mathbb{R}^{m \times m}$.
- Then

$$o_{t} = W_{hh}h_{t-1} + W_{hx}x_{t} + b_{h}$$

$$h_{t} = \tanh(o_{t}) = \tanh(W_{h} \cdot [h_{t-1}, x_{t}] + b_{h})$$

$$y_{t} = g(W_{y}h_{t} + b_{y})$$

for some activation function g.

• We can show that

$$\nabla_{W_{hh}}(h_t) = \sum_{t'=1}^{t-1} h_{t'} \left(W_{hh}^{t-t'-1} \tanh'(o_{t'+1}) \cdot \dots \cdot \tanh'(o_t) \right).$$

So the influence of $h_{t'}$ on h_t will be small if $t' \ll t$ as $\tanh(x)$ is small for |x| > 2, i.e., we have a vanishing gradient problem.

3.2 LSTM

- Introduce cell state to RNN.
- Information is added or removed to the cell state through gates.
- Forget gate:
 - Input: previous cell state C_{t-1} and x_t .

- Output: number in [0,1] for each entry in C_{t-1} , i.e., how much to forget.
- So we have

$$f_t = \sigma(W_{hf}h_{t-1} + W_{xf}x_t + b_f)$$

= $\sigma(W_f \cdot [h_{t-1}, x_t] + b_f),$

where σ is the sigmoid function applied element-wise.

• Input and update gate:

- Decide what and how much to add to the cell state.
- What to add:

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C).$$

- How much to add:

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i).$$

- Update cell state:

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$

where \odot is element-wise multiplication.

• Output gate:

- Decide what parts of cell state to output:

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o).$$

- Actual output:

$$h_t = o_t \odot \tanh(C_t)$$

• Drawbacks: computational complexity, overfitting, dropout harder to implement, sensitive to different random weight initializations, inability to handle temporal dependencies that are longer than a few steps,

3.3 Seq2seq

- Input \rightarrow Encoder \rightarrow Context Vector \rightarrow Decoder \rightarrow Output
- Encoder and decoder are both RNNs or LSTMs.
- Last hidden state of encoder is context vector, which initializes decoder RNN.
- At each time step, decoder receives previous token (input of RNN) and uses previous hidden state. The output of RNN is fed though FNN to get embedding of word.
- Stop when EOS token is outputted.
- For back-propagation, *teacher forcing* is used, i.e., plug in correct words to decoder and stop at correct length.
- Drawbacks:
 - Bottleneck problem: for long input sequences, information would tend to be lost.
 - For the decoder, different information may be relevant at different steps.

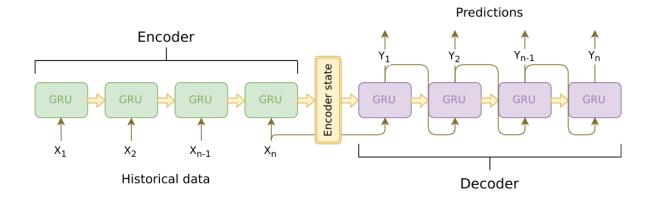


Image source: [5]

3.4 Seq2seq with Attention

- At each decoder step, it decides which source parts are more important
- Concretely, at each t,:
 - (i) Use previous token in RNN to update hidden state h_t .
 - (ii) Compute score(h_t, s_k) between decoder hidden state h_t and all encoder hidden states s_1, \ldots, s_m ;
 - (iii) Compute attention weights: softmax attention scores;
 - (iv) Compute attention vector a_t : weighted sum of encoder states.
 - (v) Use attention vector a_t and hidden state h_t in FNN to get output token.
- Popular score functions:
 - Dot-product: $score(h_t, s_k) = h_t^T s_k$.
 - Bilinear function: $score(h_t, s_k) = h_t^T W s_k$.
 - Multi-layer perceptron: $score(h_t, s_k) = v^T \tanh(W[h_t, s_k]).$
- Drawback: RNN is difficult to parallelize.

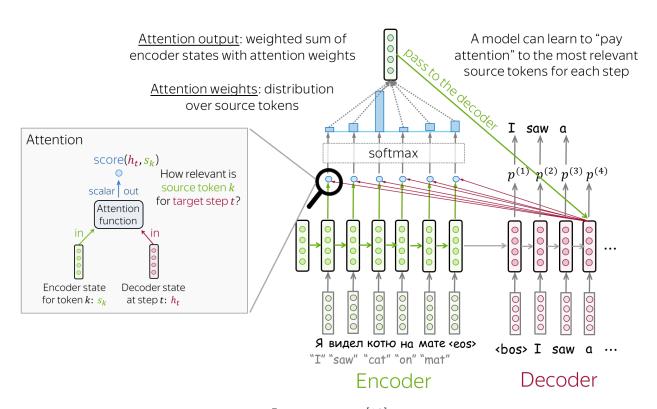


Image source: [12]

Transformers

- Encoding component is a stack (six in original paper) of encoders with same structure but different weights. Decoding component is a stack of decoders of the same number.
- Encoders: Self-Attention \rightarrow FNN
 - First encoder receives embedding of words.
 - Other encoders receive output of encoder directly below.
- Decoders: Self-Attention \rightarrow Encoder-Decoder Attention \rightarrow FNN

4.1 Ingredients

4.1.1 Self-attention

Process:

- 1. Create three vectors from each of the encoder's input vectors: Query, Key, and Value vectors.
- 2. Note: in original paper, input vectors are in \mathbb{R}^{512} , and QKV vectors are in \mathbb{R}^{64} .
- 3. Self-attention score between i-th and j-th word is $q_i \cdot k_j$ for all j.
- 4. Divide scores by square root of dimension (8; this gives more stable gradients) and softmax.
- 5. Multiply each value vector v_i by softmax scores.
- 6. Sum up the weighted value vectors. This is output of self-attention layer for i-th word.

In matrix form, suppose our input is $X \in \mathbb{R}^{n \times d}$, where n is the sequence length and d is the embedding dimension. (So rows of X are the inputs.) The QKV matrices are given by $W_Q, W_K, W_V \in \mathbb{R}^{d \times d_k}$. Then the QKV vectors

$$Q = XW_Q$$
$$K = XW_K$$
$$V = XW_V$$

are in $R^{n \times d_k}$ For each attention head, we have

$$\operatorname{Attention}(Q,K,V) = \operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) \times V \in \mathbb{R}^{n \times d_k},$$

i.e., aggregate values weighted by attention.

4.1.2 Multi-headed attention

Do h parallel attention heads, with different weight matrices for each head.

$$MultiHead(Q, K, V) = Concat(head_1, ..., head_h) \times W_O$$

where

$$head_i = Attention(Q_i, K_i, V_i)$$

is output of each attention head and $W_O \in \mathbb{R}^{hd_k \times d}$. Note that MultiHead $(Q, K, V) \in \mathbb{R}^{n \times d}$.

4.1.3 Positional encoding

Transformers are permutation-invariant, so we add positional encoding to input embeddings.

4.1.4 FNN

Output of attention fed into FNN:

$$FNN(x) = ReLU(xW_1 + b_1)W_2 + b_2.$$

4.1.5 Residual connections & layer normalization

Each sub-layer (attention or feedforward) is followed by

$$LayerNorm(x + Sublayer(x)).$$

Given $x \in \mathbb{R}^d$, the layer norm is

$$LayerNorm(x) = \frac{x - \mu}{\sqrt{\sigma^2 + \epsilon}} \cdot \gamma + \beta,$$

where

$$\mu = \frac{\sum x_i}{d} \text{ (mean over features)}$$

$$\sigma^2 = \frac{\sum (x_i - \mu)^2}{d} \text{ (variance over features)}$$

 γ, β : learned scaling and shifting parameters ϵ : small constant to prevent division by zero.

4.2 Original Architecture

Encoder Layer:

- Input Embedding + Positional Encoding
- Multi-Head Self-Attention \rightarrow Residual + Layer Norm
- Feed-Forward Network \rightarrow Residual + Layer Norm

Decoder Layer:

- Masked Multi-Head Self-Attention (prevent peeking at future tokens)
- Multi-Head Encoder-Decoder Attention \rightarrow Residual + Layer Norm
- Feed-Forward Network \rightarrow Residual + Layer Norm

4.3 Modern Architecture

- Input Embedding
- Layer Norm \rightarrow Self-Attention \rightarrow Residual
 - Grouped-Query Attention
 - Rotary Embeddings
- Layer Norm \rightarrow FNN \rightarrow Residual

4.3.1 Grouped-query attention

- Use same W_K and W_V across heads, and each head has its own W_Q .
- Better: divide heads into groups. Heads in the same group share W_K and W_V

4.3.2 Rotary positional embeddings (RoPE)

- Limitations of absolute positional embedding:
 - Limited sequence length
 - Independence of positional embedding, e.g./ difference between position 1 and 2 is the same as the difference between position 1 and 500
- Alternative: relative positional embeddings [10]
 - Bias for positional offsets: use a bias to represent each possible positional offset
 - Relative attention becomes:

Attention
$$(Q, K, V)_i = \sum_{j=1}^n \operatorname{softmax}(e_{ij}) \times (x_j W_V + a_{ij}^V),$$

where

$$e_{ij} = \frac{QK^T + x_i W_Q(a_{ij}^K)^T}{\sqrt{d_{ij}}}.$$

- Here, $a_{ij} \in \mathbb{R}^{1 \times d_a}$ is a vector of relative positional weights, i.e.,

$$a_{ij} = w_{\text{clip}(j-i,k)}$$
$$\text{clip}(x,k) = \max(-k, \min(k, x)).$$

Calculate w for both keys and values.

- Clipping allows scalability (i.e., arbitrarily long sequences)
- Limitations: slower; complicates key-value cache usage as each additional token changes the embedding for every other token.
- For RoPE [11], the intuition is to rotate each embedding by $m\theta$, where m is the position of the word in the sequence.
- Benefits:

- Scalability: adding new words does not change the embedding of previous words
- The dot product of the embeddings of two words does not depend on absolute position.
- Mathematically, we first work in $\mathbb{C}^{d_k/2}$. Let M_j be the rotation matrix by $m\theta_j$. Then the output of RoPE for the m-th word is just

$$Q_m\Theta_m = Q_m imes egin{pmatrix} M_1 & & & & \\ & M_2 & & & \\ & & \ddots & & \\ & & & M_{d_k/2} \end{pmatrix},$$

where Q_m is the m-th row of Q (i.e., query vector for m-th word).

• Do the same for key vector.

4.4 Other Techniques

4.4.1 Sparse attention

Instead of global autoregressive self-attention, use local autoregressive self-attention in some layers.

4.4.2 Mixture of experts (MOE)

- Instead of a single monolithic feedforward layer in the transformer block, use a set of expert networks, and route the input to only a few of them.
- A router (a smaller FNN) calculates which experts to turn on.
- Could do model merging by doing a weighted average of experts using weights from the router.

Fine-Tuning Techniques

Full fine-tuning, of course, has the best performance but is computationally expensive. Need parameter-efficient fine-tuning (PEFT).

- Adapter-based methods
 - Adapters: small, trainable models inserted into pre-trained transformers.
 - Freeze original model weights.
- Instruction tuning

5.1 Low-Rank Adaptation (LoRA)

Introduced in [8].

- Intuition: only train low rank perturbations of the (selected) weight matrices.
- Let $W_0 \in \mathbb{R}^{d \times k}$ be a pre-trained weight matrix.
- Update: $W_0 + \Delta W = W_0 + BA$, where $B \in \mathbb{R}^{d \times r}, A \in \mathbb{R}^{r \times d}, r \ll \min(d, k)$.
- Advantages:
 - Roughly converges to full fine-tuning as r increases.
 - No additional inference latency: when needing to switch to another downstream task, can recover W_0 by subtracting BA, and then we can add a new B'A'.
- Notes [6]:
 - Optimal placement highly dependent on the dataset and model architecture.
 - For transformers, applying LoRA exclusively to attention layers provides the most stability and mitigates the risk of divergence.
 - For MoE, applying LoRA to each expert individually boosts performance, but significantly increases memory usage. Applying to router gives limited success.
 - Could optimize memory by using same B across different A.

5.2 QLoRA

Quantized LoRA, introduced in [4].

5.2.1 4-bit NormalFloat Quantization

- Better quantization data type for normally distributed data.
- In general, for k-bit Normal Float, equally divide the normal distribution into 2^k quantiles.
- Note: to ensure 0 has an exact representation, actually divide the negative part into 2^{k-1} quantiles and the positive part into $2^{k-1}+1$ quantiles, then remove one of the two overlapping zeros.
- Then

$$X^{\mathrm{NF4}} = \mathrm{round}\left(\frac{1}{\mathrm{absmax}(X^{\mathrm{FP32}})}X^{\mathrm{FP32}}\right) = \mathrm{round}(c^{\mathrm{FP32}}X^{\mathrm{FP32}}),$$

where c^{FP32} is the quantization constant.

5.2.2 Block-wise Quantization

- One problem is quantization is that outliers severely impacts the scaling, and the full range of the lower precision data type may not be effectively used.
- Solution: Chunk the input tensor into blocks that are independently quantized, each with its own quantization constant.

5.2.3 Double Quantization

- Helps reduce the memory footprint of quantization constants.
- Block-wise k-bit quantization for the quantization constants c^{FP32} .
- Gives $c_2^{k\text{-bit}}$, with second level of quantization constants c_1^{FP32} .

5.2.4 Implementation

• Recall: LoRA has

$$Y = XW + XL_1L_2$$

for low rank matrices L_i .

• For QLoRA, do

$$Y^{\rm BF16} = X^{\rm BF16} \, {\rm double Dequant}(c_1^{\rm FP32}, c_2^{k\text{-bit}}, W^{\rm NF4}) + X^{\rm BF16} L_1^{\rm BF16} L_2^{\rm BF16},$$

where

$$\operatorname{doubleDequant}(c_1^{\operatorname{FP32}}, c_2^{k\operatorname{-bit}}, W^{\operatorname{NF4}}) = \operatorname{dequant}(\operatorname{dequant}(c_1^{\operatorname{FP32}}, c_2^{k\operatorname{-bit}}), W^{\operatorname{NF4}}) = W^{\operatorname{BF16}}(c_1^{\operatorname{FP32}}, c_2^{k\operatorname{-bit}}) = W^{\operatorname{BF16}}(c_1^{\operatorname{FP32}}, c_2^{k\operatorname{-bit}})$$

- Original paper [4] uses FP8 for c_2 , block size of 64 for W, and block size of 256 for c_2 .
- Computations done in BF16 and storage of W in NF4.

Fourier Transform

• Let x(t) be a complex-valued function. Then its Fourier transform is

$$X(\omega) = \int_{-\infty}^{\infty} x(t)e^{-i\omega t} dt.$$

The inverse Fourier transform is

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} X(\omega) e^{i\omega t} d\omega.$$

• For a sequence of discrete time signals, use discrete-time Fourier transform:

$$X(\omega) = \sum_{-\infty}^{\infty} x[n]e^{-i\omega n}.$$

The output is continuous in ω and periodic. The inverse DTFT is:

$$x[n] = \frac{1}{2\pi} \int_{2\pi} X(\omega) e^{i\omega n} d\omega.$$

• Discrete Fourier transform converts a finite sequence of equally-spaced samples of a function into a same-length sequence of equally-spaced samples of the DTFT. It is given by

$$X[k] = \sum_{n=0}^{N-1} x[n]e^{-2\pi i k n/N}$$
$$= \sum_{n=0}^{N-1} x[n]W_N^{kn},$$

where $W_N = e^{-2\pi i/N}$. The inverse transform is given by

$$\frac{1}{N} \sum_{k=0}^{N-1} X[k] W_N^{-kn}.$$

• The fast Fourier transform is based on the idea that the N-th roots of unity W_N^k have nice properties when N is a power of 2. In vector form,

$$\mathbf{X}[k] = \mathbf{W_N} \mathbf{x}[n],$$

where $W_N = V(W_N^0, \dots, W_N^{N-1})$ is a Vandermonde matrix. The computational complexity is $O(N \log N)$ vs. $O(N^2)$ of definition of DFT.

- Limitation of Fourier transform is that it lacks temporal resolution. A way to overcome this is the short-time Fourier transform.
 - Continuous case:

$$STFT\{x(t)\}(\tau,\omega) = \int_{-\infty}^{\infty} x(t)w(t-\tau)e^{-i\omega t} dt,$$

where w is the window function, usually Hann or Gaussian window.

- Discrete case:

$$STFT\{x[n]\}(k,\omega) = \sum_{n=-\infty}^{\infty} x[n]w[n-k]e^{-i\omega n}.$$

Uncertainty principle: there is a trade-off between temporal and frequency resolution.

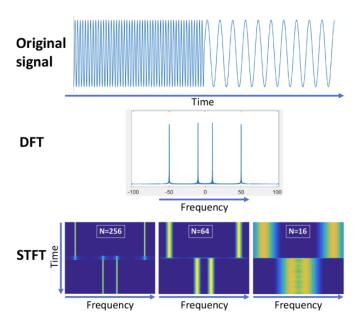


Image source: [7]

• Spectrograms:

- Divide a time-domain signal into segments of equal length.
- Apply FFT to each segment, transforming the data from the time domain to the frequency domain.
- Each segment corresponds to vertical line in spectogram.
- For window width w, spectogram $(t) = |\operatorname{STFT}(t)|^2$.
- Nyquist-Shannon sampling theorem
 - Sampling rate must be at least twice the bandwidth of the signal to avoid aliasing.
 - Let x(t) have Fourier transform X(f). Suppose $X_{1/T}(f)$ is the DTFT of sample sequence x[n].
 - For DTFT, copies of X_f are shifted by multiples of the sampling rate f_s and added.

- $-\,$ If Nyquist–Shannon is not satisfied, copies will overlap.
- Any frequency component above $f_s/2$ is indistinguishable from a lower-frequency component (i.e., alias).

Bibliography

- [1] Jay Alammar. Online Blog. https://jalammar.github.io/.
- [2] Jay Alammar and Maarten Grootendorst. How Transformer LLMs Work. Online Course. https://www.deeplearning.ai/short-courses/how-transformer-llms-work.
- [3] Aziz Belaweid. Complete Summary of Absolute, Relative and Rotary Position Embeddings! Online Blog. https://azizbelaweid.substack.com/p/complete-summary-of-absolute-relative.
- [4] Tim Dettmers, Artidoro Pagnoni, Ari Holtzman, and Luke Zettlemoyer. Qlora: Efficient finetuning of quantized llms, 2023.
- [5] Joseph Eddy. Forecasting with Neural Networks An Introduction to Sequence-to-Sequence Modeling Of Time Series. https://jeddy92.github.io/ts_seq2seq_intro/.
- [6] Vlad Fomenko, Han Yu, Jongho Lee, Stanley Hsieh, and Weizhu Chen. A note on lora, 2024.
- [7] Diego Hernando. Lecture 16: Limitations of the Fourier Transform: STFT. Mathematical Methods in Medical Physics Lecture Notes, April 2016. https://qiml.radiology.wisc.edu/wp-content/uploads/sites/760/2022/12/notes_016_STFT.pdf.
- [8] Edward J. Hu, Yelong Shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, and Weizhu Chen. Lora: Low-rank adaptation of large language models. CoRR, abs/2106.09685, 2021.
- [9] Neil Laws. Part A Statistics. Lecture Notes, April 2016.
- [10] Peter Shaw, Jakob Uszkoreit, and Ashish Vaswani. Self-attention with relative position representations. *CoRR*, abs/1803.02155, 2018.
- [11] Jianlin Su, Yu Lu, Shengfeng Pan, Bo Wen, and Yunfeng Liu. Roformer: Enhanced transformer with rotary position embedding. *CoRR*, abs/2104.09864, 2021.
- [12] Lena Voita. Sequence to Sequence (seq2seq) and Attention. NLP Course. https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html.