General ML Concepts

- Initialization
  - Zero vs. Random
    - Zero -> cannot learn well -> outputs of all neurons are same -> weight updates be same -> can represent one/limited number of features -> required randomness
    - Random -> vanishing/exploring gradient if random values are very low/high.
  - He vs. Xavier/Glorot
    - $\text{He}: \mu = 0, \sigma = \sqrt{2/n_{in}}$ and $\text{Xavier}: \mu = 0, \sigma = \sqrt{2/(n_{in} + n_{out})}$
    - $\sigma_{he}^2 > \sigma_{xav}^2 \rightarrow$ He is more prone to operate in saturated region for symmetric activation function. So, Xavier is more suitable for sigmoid/tanh, while He is for ReLU.
    - Having both n_{in} and n_{out} in Xavier makes the variance balanced/symmetric for forward and backward passes that makes it suitable for symmetric activation functions.
    - He is tailored for ReLU. Variance is preserved for inputs in all layers that ensures a stable gradient flow and thus avoid vanishing gradient problems.
      - $\text{Var}(WX) = \sum \text{Var}(W_iX_i) = \sum \text{Var}(W_i)\text{Var}(X_i) = n_{in} * \frac{2}{n_{in}} * \sigma_x^2 = 2\sigma_x^2$
      - $\text{Var}(\text{ReLU}(WX)) \approx \frac{1}{2}\text{Var}(WX) = \frac{1}{2} * 2\sigma_x^2 = \sigma_x^2 \rightarrow \text{variance preserved}$
    - Reduced variance for Xavier with ReLU implies that it's more prone to vanishing gradient. However, reduce variance for Xavier with Sigmoid helps to keep inputs within the linear range.
      - $\text{Var}(WX) = \sum \text{Var}(W_iX_i) = \sum \text{Var}(W_i)\text{Var}(X_i) = n_{in} * \frac{2}{n_{in}+n_{out}} * \sigma_x^2 = \frac{2}{1+\frac{n_{out}}{n_{in}}}\sigma_x^2$
      - $\text{Var}(\text{ReLU}(WX)) \approx \frac{1}{2}\text{Var}(WX) = \frac{1}{2} * \frac{2}{1+\frac{n_{out}}{n_{in}}}\sigma_x^2 = \frac{\sigma_x^2}{1+\frac{n_{out}}{n_{in}}} \rightarrow \text{variance reduced}$
    - He is more prone to vanishing gradient when used with Sigmoid (because of high σ_{he}^2), and Xavier is more prone to vanishing gradient when used with ReLU (because of reduced σ_x^2).
- Activation function
  - Required to introduce non-linearity and therefore, to capture complex patterns.
  - Sigmoid (for binary class probabilities), Tanh (when data needs to be centered around zero), Softmax (for multiclass probabilities), ReLU, Leaky ReLU, GeLU. At $x = 0$, use $\nabla\text{ReLU} = 0$.
  - For multi-label multi-class problems use Sigmoid separately for each output neuron.
- Cost function
  - Properties of good cost functions: Convex, continuous, differentiable. If not differentiable at any x, use 0.
  - Cross-Entropy loss is commonly used as cost function in classification tasks, and is widely used because:
    - CE is convex, continuous, differentiable for classification.
    - CE measures the difference between two probability distributions by taking the negative log-likelihood of the true labels given the predicted probabilities (that we want in classification).
      - $H(P, Q) = -\sum P(y)\log Q(y) = -y\log\hat{y} - (1-y)\log(1-\hat{y})$
  - KL-Divergence: Commonly used to measure how one probability distribution diverges from another.
    - $D_{KL} = \sum P\log\frac{P}{Q} = \sum P(\log P - \log Q) = \sum P\log P - \sum P\log Q = H(P, Q) - H(P)$
    - $H(P)$: Entropy of P; measures the inherent uncertainty/randomness in true distribution P.
    - $H(P, Q)$: Cross-Entropy; measures total uncertainty when approximating P by Q.
    - $H(P, Q) - H(P)$: KL Divergence; measures additional uncertainty introduced by Q.

- Cost functions in linear and logistic regressions: MSE vs. CE
  - MSE loss is for linear regression and cross-entropy loss is for logistic regression.
  - Linear regression assumes a normal distribution of error, and MSE aligns with this assumption, while logistic regression assumes a binomial distribution of the output, and cross-entropy aligns with this assumption.
  - Both MSE and CE are convex functions. Second derivative of convex functions is positive.
    - $\mathrm{MSE} \approx (y - XW)^2 \rightarrow \nabla^2 = X^2$
    - $\mathrm{CE} = -y \log p - (1-y)\log(1-p) \rightarrow z(1-y) + \log(1+e^{-z}) \rightarrow \nabla^2 = e^{-z}/(1+e^{-z})^2$
  - MSE cannot be used for logistic regression because of two reasons:
    - The assumptions do not align.
    - MSE for logistic regression can become non-convex since it involves squaring of a non-linear logistic function. $\mathrm{MSE}_{\text{logistic}} \approx (y-p)^2 = \nabla^2$, which can be negative for some θ.
  - CE specifically designed for classification tasks and is not suitable to continuous outputs.
  - Use MLE to estimate parameters in logistic regression, while use OLS for linear regression. OLS is equivalent to MLE for linear regression, because of normality assumption of the residuals.

$$\epsilon \sim N(0,\sigma^2) \approx Y \sim N(X\hat{\beta},\sigma^2) = N(\hat{Y},\sigma^2)$$

$$\text{lik } Y = \prod_{i=1}^{n} N(\hat{Y}_i,\sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(Y_i-\hat{Y}_i)^2}{2\sigma^2}\right)$$

$$\log \text{lik } Y = n * \log\frac{1}{\sqrt{2\pi\sigma^2}} - \sum_{i=1}^{n}\frac{(Y_i-\hat{Y}_i)^2}{2\sigma^2} = n * \log\frac{1}{\sqrt{2\pi\sigma^2}} - \frac{n}{2\sigma^2} - \sum_{i=1}^{n}(Y_i-\hat{Y}_i)^2$$

$$\max \log \text{lik } Y \approx \min \sum_{i=1}^{n}(Y_i-\hat{Y}_i)^2$$

- Parameter Estimation: MLE vs. MAP
  - MLE seeks for params that maximize the likelihood $\mathbf{L}(\boldsymbol{\theta}|\mathbf{x})$ (or equivalently the probability $\mathbf{P}(\mathbf{x}|\boldsymbol{\theta})$), while MAP seek for params that maximize posterior probability: $\mathbf{P}(\boldsymbol{\theta}|\mathbf{x}) \propto \mathbf{L}(\boldsymbol{\theta}|\mathbf{x}) * \mathbf{P}(\boldsymbol{\theta})$.

$$\hat{\boldsymbol{\theta}}_{\mathbf{MLE}} = \underset{\boldsymbol{\theta}}{\mathbf{argmax}}\, \mathbf{L}(\boldsymbol{\theta}|\mathbf{x})$$

$$\hat{\boldsymbol{\theta}}_{\mathbf{MAP}} = \underset{\boldsymbol{\theta}}{\mathbf{argmax}}\, \mathbf{L}(\boldsymbol{\theta}|\mathbf{x}) * \mathbf{P}(\boldsymbol{\theta})$$

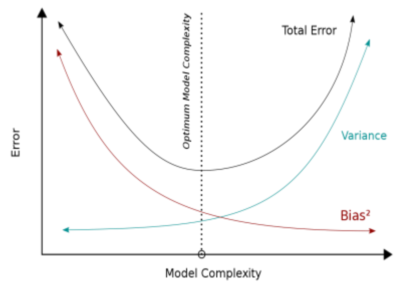
  - Both MLE and MAP are used for parameters estimation; but MLE does not consider any prior distribution over the parameters (purely data-driven), while MAP uses a prior, aligning with Bayesian principles.
  - During model training, MLE is used to minimize a likelihood-based loss function. MAP is implicitly used in regularization: L1 assumes Laplace distribution and L2 assumes Gaussian distribution over the params.
    - $L = (y-\hat{y})^2 + \lambda\|w\|_k$ where $k = 1$ for L1 or $k = 2$ for L2 regularization.
    - L2-norm is linked to Gaussian, while L1-norm is linked to Laplacian distributions, i.e., negative log-likelihood of Gaussian is proportional to L2-norm and negative log-likelihood of Laplacian in proportional to L1-norm.

$$G = c\exp(-\gamma(x-\mu)^2) \rightarrow \log G = \prod_{i=1}^{n} c\exp(-\gamma(x-\mu)^2) \rightarrow -\log G = -n\log c + \gamma\sum_{i=1}^{n}(x-\mu)^2$$

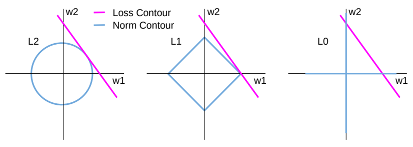
$$L = c\exp(-\gamma|x-\mu|) \rightarrow \log L = \prod_{i=1}^{n} c\exp(-\gamma|x-\mu|) \rightarrow -\log L = -n\log c + \gamma\sum_{i=1}^{n}|x-\mu|$$

- Backpropagation
  - An algorithm or process of updating weights based on the derivatives of cost function.
  - Compute the gradient of the loss function w.r.t. the params using chain rule and update the params.

- Optimizer
  - Gradient descent, SGD: Gradient is rate of change -> we want to go in the direction with maximum change, i.e., to the steepest direction -> take the directional derivative to find that direction -> $\nabla_{\hat{u}} f = \nabla f(x) . \hat{u} = |\nabla f(x)||\hat{u}| \cos\theta = |\nabla f(x)| \cos\theta$ -> which is maximum when $\theta = 0$, and the max rate of change is $|\nabla f(x)|$ -> which implies the max is in the direction of derivative -> In gradient descent, we need to go downhill, so use negative sign in the weight update formula.
  - SGD: slower convergence, unstable; faster computes per iteration, may escape local minima because of noisy directions.
    BGD: faster convergence in terms of number of iteration required, but total compute time can be longer; stable; slower computation per iteration; more susceptible to stuck in local minima.
  - Adam uses two states:
    - SGD with momentum: First moment = mean = EMA of derivative in each weight's direction → oscillation cancelled by positive and negative → faster in other directions)
    - RMSProp: Second moment = variance = EMA of squared derivative in each weight's direction → learning rate is divided by second moment))
- Hyperparameters
  - Network architecture: Number of layers, hidden size, activation function
  - Regularization
    - Concepts: Overfitting, underfitting, and bias-variance tradeoff
      - Overfitting: Models learn training data too well, including its noises and outliers, but fail on new data → model is too complex → introduce error due to variance.
      - Underfitting: Models fail to learn enough from training data; poor performance on both training and new data → model is too simple → introduce error due to bias.
      - Bias-variance tradeoff: Find a good balance between bias and variance, minimizing total error. Total error = Bias^2 + Variance (+ irreducible errors, e.g., measurement errors)
      - Use regularization (e.g., L1, L2, dropout), ensembles, normalization, data augmentation to overcome overfitting.

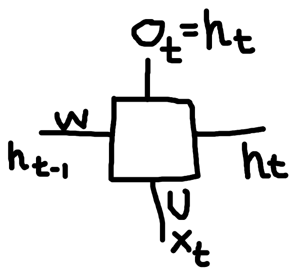


    - L2 vs. L1 vs. L0 regularization
      - L_2 reduces the magnitudes of weights. $w_i = w_i - \partial C = w_i - \partial L - 2\lambda w_i = (1-2\lambda) w_i - \partial L \rightarrow$
        w_i is changed by a percentage that never become
      - L_1 sets some weights to zero. $w_i = w_i - \partial C = w_i - \partial L - \lambda * \text{sign}(x) = (w_i \pm \lambda) - \partial L \rightarrow$
        w_i is reduced by a contant that can make it 0.
      - L_0 is non-convex.



    - Dropout: Exclude some neurons/parameters during training
      - Training: scale the output of the neurons by $1/(1-p_{dropout})$
      - Testing: Use the full network with no dropping.

        - Normalization → Consistent input distribution, avoid exploding/vanishing gradients, reduce sensitivity to initialization (batch normalization vs. layer normalization)
            - Batch: Normalizes the inputs to a layer for each mini batch → depends on batch size; suitable for: larger input sizes, consistent batch statistics; so used in CNNs.
            - Layer: Normalizes the outputs of each neuron using the outputs of all neurons in that layer → used predominantly in RNNs.
            - Scaling and shifting: Normalization makes the input distribution more consistent. However, if normalization always results in mean=0 and variance=1, the network might be unable to represent data that naturally have a different distribution. Scaling and shifting after normalization helps overcoming this issue: $x_i = \gamma . \frac{x-\mu}{\sigma} + \beta$
            - Normalization during testing: Use the same normalization parameters used in training, except for layer normalization, in which normalize the output regardless of inputs.
        - Data scaling vs. data normalization
            - Scaling (-1, 1), normalization (mu=0, sigma=1) → scaling is good for distance-based models, e.g., SVM and KNN → if one feature has a larger scale than the others, it will dominate in the margin calculations.
    - Optimization/training related hyper-parameters
        - Learning rate (high (faster convergence, low stability) vs. low (slow convergence, high stability))
        - Epoch vs. batch vs. iterations (in each iteration, weights are updated for one batch)
        - Low Rank Adaptation (hyper-parameter: rank) $W = W + W_r = W + AB$
- CNN
    - Layers: input, convolution, activation, pooling, fully connected.
    - Convolution operation: A kernel/filter sliding over the input and producing a dot product.
        - Filters work as feature detectors, e.g., edges, corners, blobs, etc.
        - Dot product computes the similarity, i.e., part of the image is like the filter.
    - Pooling: Max and average pooling → used for dimensionality reduction → may help to reduce noise.
    - Concept of padding and stride? What is padding used for?
        - Padding: Ensures no border information is lost during convolution.
        - Stride: Step size of convolution filer's move → affects the spatial dimension of the output.
        - H x W x D → H' x W' x N, where H' = (H – F + 2*P) / S) + 1
        - H=height, W=width, D=depth, P=padding, S=stride, F=filter size, N=filter number.
- RNN
    - Sequential processing
    - Hidden state: Captures info processed so far → works as network's memory.
    - Challenge: vanishing gradient
        - Hidden state outputs at time point 2 and 1 are:
        - $h_2 = \sigma(Wh_1 + Ux_2) = \sigma(z_2),\ h_1 = \sigma(Wh_0 + Ux_1) = \sigma(z_1)$
        - $\frac{\partial h_2}{\partial W} = \frac{\partial h_2}{\partial h_1} . \frac{\partial h_1}{\partial W} = \frac{\partial h_2}{\partial z_2} . \frac{\partial z_2}{\partial h_1} . \frac{\partial h_1}{\partial z_1} . \frac{\partial z_1}{\partial W} = \sigma'(z_2) W \sigma'(z_1) W = W^2 \sigma'(z_2) \sigma'(z_1)$



    - LSTM: Overcomes vanishing gradient problem using gating mechanisms, making it easier to remember the long-term dependencies. **Cell state** stores the information; **forget gate** determines what info can be discarded from the cell state; **input gate** decides what new information to add in the cell state; **output gate** decides which information to take from cell state to generate output.

- NLP
    - Text processing: Tokenization, stemming & lemmatization, punctuations and stop words removal.
    - Token embeddings:
        - **One-hot-encoding**: Create a list of words present in all documents. For each sentence, put 1 for a word if that word in present in that sentence (regardless of number of frequency of the word).
        - **Label encoding**: Assign a random number for each category (Red=0, Green=1, Blue=2)
        - **Target encoding**: Take target into account. Red = target_mean_Red -> Data leakage → variants: weighted target encoding, K-fold target encoding
        - TF-IDF: Like one-hot-encoding but it considers the number of frequency of the word in the sentence, which is term frequency. Then it computes IDF and finally TF * IDF = TF * log(N/n) → N=total documents, n = document where the word is present)
        - Example: 2 sentences – I like Apple. Apple is good. → Processing → like apple. apple good.

Word level encoding

Tokens	Words		
	like	apple	good
like	1	0	0
apple	0	1	0
good	0	0	1

Sentence level encoding

Tokens	Words		
	like	apple	good
i like apple	1	1	0
apple is good	0	1	1

Sentence level TF-IDF

Tokens	Words		
	like	apple	good
i like apple	1	0	0
apple is good	0	0	1

        - Word2Vec
            - What is Word2Vec? How does it work and what are its limitations?
                - NN-based model -> learn to generate embeddings of the words in a sentence -> considers only the local context (e.g., “I like eating apple” and “apple released iPhone” have different contexts for apple, so the embeddings will be different) -> cannot capture the context when words have same local context but different meaning (e.g., “I like apple fruit” and “I like apple products” -> show affection for apple, i.e., same context -> generate same embedding for apple although their meanings are different) -> Also it does not consider the order of the words in the sentence.
            - Two architectures of word2vec
                - CBOW: Continuous bag of words -> predict the target words given context words.
                - Skip-gram -> predict the context words given the target word.

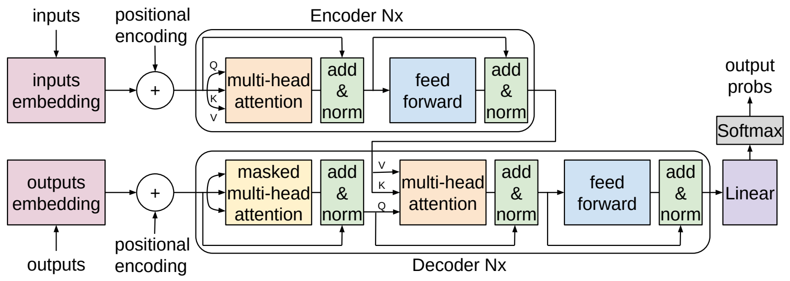
CBOW	Skip-gram
(In → out): like, apple → I	(In → out): I → like, apple
(In → out): I, apple → like	(In → out): like → I, apple
(In → out): I, like → apple	(In → out): apple → I like
The NN model learn the vector reprecipitations of the input and outputs words, so that the probability of observing the output words is maximized given the input words.	

        - Transformer-based encoding
            - Context-aware embeddings that considers the position/order of the words in the sentence.
        - How to evaluate the quality of the embeddings?
            - Performance of the downstream tasks
    - Common NLP tasks: Sentiment analysis; Named entity recognition; Parts of speech tagging; Machine translation; Speech recognition.

- LLMs
    - Foundation model: the pre-trained base model.
    - Pretraining: The foundation model is trained with a large amount and varieties of text data.
    - Optimize LLM for specific applications:
        - Fine-tuning: Further tune for specific task with limited and domain specific dataset.
        - RAG: Models first retrieves from a dataset and then use that context to generate responses.
    - Neural scaling law: Performance tends to increase with model size (parameters) and training dataset size.
    - Evaluation: Exact matching, BLEU, ROUGE, METEOR, BERTScore, Human review (accurate, complete, coherent, consistent, desired, undesired)
    - RLHF: is a training approach where the models learn the desired behavior based on feedback from human interactions, rather than solely relying on pre-collected datasets.
    - Bias

	Data	**Model**
Sources of biases	Underrepresented train data	Complex/overfitting
How to measure biases?	Statistics: Proportion & Distribution Metrics (e.g., accuracy) per category	Stability analysis: Introduce noise in inputs → Small input changes results in larger output shifts
How to remediate biases?	Resampling Data augmentation	Regularization Multi-objective optimization

- **Transformer**
    - Fundamentals: Input embedding, positional encoding, self-attention mechanism, multi-head attention, masked multi-head attention, layer normalization, residual connection, output probabilities, sampling, sources of variability in generation.



$$\mathrm{Attention}(Q, K, V) = \mathrm{Softmax}\left(\frac{Q.K^T}{\sqrt{d_k}}\right)V$$

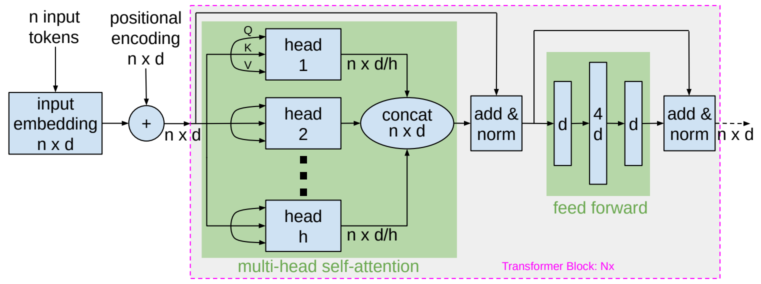
    - Q: what context is represented by a word? K: how each word is related to the Q word? V: represents the content; it helps the model to understand and interpret the sentence. Analogy: Let's we're interested to retrieve information about a topic in a book. Have a topic/context in mind → go to the index and find the most similar one → go to the indexed page and retrieve the content.

Q=Topic interested in, K=Book index, V=Content at indexed page.

    - Limitations (remedy): memory-intensive (weight quantization), resource-intensive (knowledge distillation), scalability of self-attention (use sparse attention patterns)
    - Handling multimodal inputs: Joint embedding and then general self-attention; dedicated encoding layers for each modality and combine their representations; cross-modal attention mechanism.

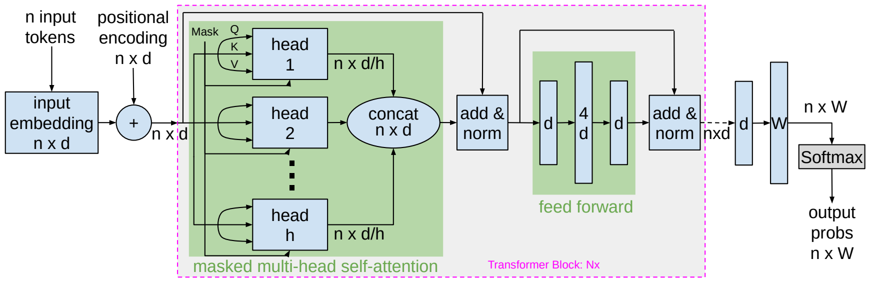
$$\mathrm{CrossModalAttention}(Q_{text}, K_{image}, V_{image}) = \mathrm{Softmax}\left(\frac{Q_{text}.K_{image}^T}{\sqrt{d_{k,image}}}\right)V_{image}$$

    - Cross-modal attention mechanism, dedicated encoding layers for each modality, joint embedding space.
    - Responsible AI: Bias, misinformation, privacy; enhance interpretability by attention weights visualization.
- **BERT: d = 768, h = 12, Nx = 12**

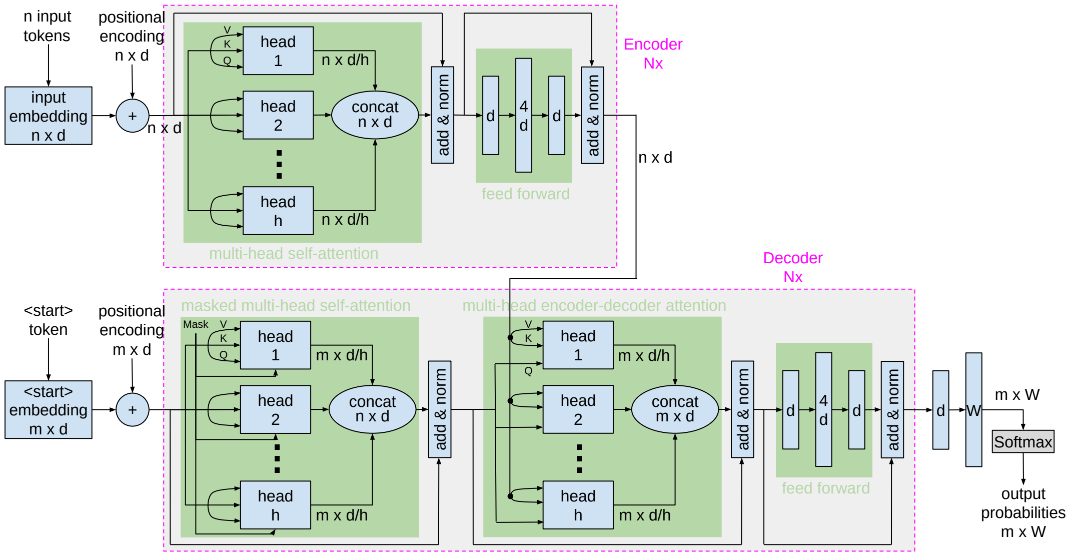


    - Uses only the encoding mechanism of transformer and is suitable for tasks related to understand context.
    - Inputs (max 512 embeddings for base and 1024 embeddings for large model)
        - [CLS] + (n-1) tokens → input embeddings + position embeddings
    - Training: Multi-task learning -> Task 1: Masked Language Model (MLM, 15% of words are masked), and Task 2: Next Sentence Prediction (NSP, 50% of the second sentences are actual second sentences and the remaining 50% of the second sentences are randomly chosen from corpus).
        - Two pre-trained versions (L = #attention layer, A = #heads, H=hidden layer size)
            - BASE (L=12, A=12, H=768; Total Parameters=110M)
            - LARGE (L=24, A=16, H=1024, Total Parameters=340M)

- **GPT-3: d = 2048, h = 16, Nx = 96, W = 30k**



  - Uses only the decoding mechanism with only masked multi-head attention and is suitable for text generation tasks.
  - Input tokens -> embeddings -> decoder block (multi-head self-attention, position-wise FFNN with layer norm and residual connections) -> Linear -> Softmax -> Probabilities of all possible words in dictionary usually 30k-50k words and pick the one with the highest probability or randomly pick one from a set of words with probabilities > threshold.
  - After generating the first output tokens, it is used with the original input tokens and generates the second output token, and so on.
- **T5/BART: d = 4096, h = 128, Nx = 24**



- **Vision Transformers**
  - **ViT vs. Swin**
    - ViT -> image patches -> transformer model -> image classification (max 197 inputs).
    - Swin Transformer -> image patches of different scales -> transformer model -> object detection / semantic segmentation (max 224 input embeddings).
  - **Oscar vs. ViLBERT**
    - Oscar -> Object-Semantics Aligned Pre-training -> image embeddings and text embeddings -> same transformer model -> cross-modal attention-> decoder -> generate text caption of the image (max 74 input embeddings)
    - ViLBERT -> Visual Linguistic BERT -> image embeddings and text embeddings -> two-stream transformer models -> cross-modal attention -> decoder -> generate text caption of the image (max 128 input embeddings)

REGRESSION

Linear regression:

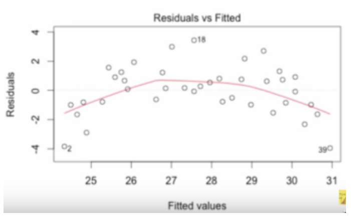
Definition: $Y = X\beta + \epsilon$, OLS solution by setting derivative of RSS to zero: $\hat{\beta} = (X^T X)^{-1} X^T y$

$$\mathrm{RSS} = (y - X\beta)^T (y - X\beta) = y^T y - y^T X\beta - \beta^T X^T y + \beta^T X^T X\beta = y^T y - 2\beta^T X^T y + \beta^T X^T X\beta \rightarrow \nabla = -2X^T y + 2\beta X^T X$$

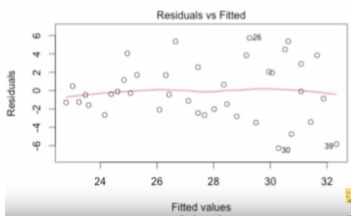
- Assumptions for linear regression:
    - Response variable is linearly related to the predictor variables. Plot normalized residuals vs. predictors. If this assumption is violated, then try to transform the data (either Y or X or both) and use them in the model. Common transformation may include log (for positive data!), X^2 etc.
    - Samples are independent.
    - Predictors are independent (no multi-co-linearity).
        - Rule of thumb: VIF > 10 reflects high co-linearity, cutoff VIF = 5.

$$\mathrm{VIF}_i = \frac{1}{1 - R_i^2}, \qquad \text{where,} \qquad R_1^2 \text{ is for } X_1 = \beta_2 X_2 + \cdots + \beta_n X_n + \epsilon$$

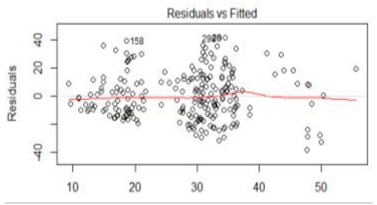
        - We can remove collinear predictors or use Ridge penalty, reduce dimensions.
    - Variances of errors are constant for all X's. Plot residuals vs. fitted values. If this assumption is not violated, then the residuals should approximately equal for all fitted values.
    - Residuals are normally distributed. Observe QQ plot or histogram of residuals to test the normality. Also k-s test or shapro-wilk test can be used.
    - For a fixed value of x, e.g., x=0, the outputs are normally distributed.
- All the above assumptions (except the linearity one) are also the assumptions for ANOVA.



Linearity assumption is violated.



Equal variance assumption is violated.

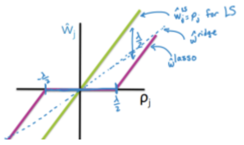


Clusters indicated multi-collinearity!

Types of linear regression:

- Simple: $Y = X\beta + \epsilon$ with p = 1 and multiple: $Y = X\beta + \epsilon$ with p > 1, polynomial: $Y = X\beta + \epsilon$ with x's powers.
- Stepwise: Forward stepwise and backward stepwise (feature selection, O(D^2) << O(2^D) for all subset method)
- Ridge: Cost with L2 penalty: $C = (y - \hat{y})^2 + \lambda |w|^2$ -- Good for prediction
    - Optimization using gradient descent: $w_j = w_j - \alpha \frac{dC}{dw_j}$, α is the learning rate.
- Lasso: Cost with L1 penalty: $C = (y - \hat{y})^2 + \lambda |w|$ -- Good for feature selection
    - If ρ_j be the derivative of RSS without jth predictor (or coordinate), Optimization using coordinate descent:

$$w_j = \begin{cases} \rho_j + \frac{\lambda}{2}, & \rho_j < -\frac{\lambda}{2} \\ 0, & \text{otherwise} \\ \rho_j - \frac{\lambda}{2}, & \rho_j > \frac{\lambda}{2} \end{cases}$$



K-Nearest Neighbor (kNN)

- Given x_{test}, find x_{train} that are closer to x_{test} (based on computed distance like eucledian, cosine, etc.). Then $y_{test} = \frac{1}{k} * (y_{train,1} + y_{train,2} + \dots + y_{train,k})$

Weighted kNN: $y_{test} = \frac{1}{w_1 + \cdots + w_k} (w_1 * y_{train,1} + \dots + w_k * y_{train,k})$, where $w_i = \frac{1}{\mathrm{distance}(x_{test}, x_i)}$, or other function, which is called the "kernel".

CLASSIFICATION

- Precision: Proportion of relevant information retrieved; Recall: Fraction of all relevant information found.
- ROC-AUC: TPR vs. FPR and PR-AUC: Precision vs. Recall.

		Predicted		
		+	-	
True	+	TP	FN (Type 2)	TPR = TP/(TP+FN) = Recall = Sensitivity

	-	FP
		(Type 1)
			TN	FPR = FP / (FP + TN)
				TNR = Specificity = TN/(TN+FP)

		PPV = Precision = TP/(TP+FP)	NPV = TN/(TN+FN)	

(1) Logistic regression

- Link function for logistic regression: sigmoid, i.e.

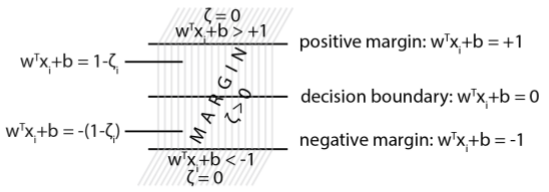
$$y = \mathrm{sigmoid}\left(-(w^T X + b)\right) = \frac{1}{1 + \exp(-(w^T X + b))} \rightarrow \; w^T X + b = \log\frac{p}{1-p} = \mathrm{logit}(p) = \mathrm{logodds}$$

- Log-odds are linear combination of the predictors and have a nice symmetric property.
  - For example, if log-odds of occurring an even = 0.2, then the log-odds of not occurring the event is -0.2.
  - Log-odds of occurring the event = logit(p)=0.2 → p = 0.55; log-odds of not occurring the event = logit(1-p)=-0.2 → 1-p=0.45, which confirms the symmetric property of the log-odds.
- Use log-loss function: $C = -\, y \log p - (1-y)\log(1-p)$
- Assumptions: (1) Independent observations (2) Response variables are binomial (2) No multi-co-linearity
- Algorithm: $X\ (mxn), Y\ (mx1)\ \rightarrow\ Z\ (mx1), A\ (mx1), C\ (mx1)\ \rightarrow\ dW\ (nx1), db\ (1x1)$
  - Initialize: $W\ (1xn)$ and $b\ (1x1)$
  - While not converged:
    - Forward propagation: (i) Linear, $Z = XW + b = np.dot(X, W)$ (ii) Activation, $A\ =\ \mathrm{sigmoid}(Z)$
    - Cost, $C\ = -\ Y \log A -\ (1 -\ Y)\log\,(1 -\ A)$
    - Backward propagation:
      - $dW = \frac{\partial C}{\partial W} = \frac{\partial C}{\partial A}\frac{\partial A}{\partial Z}\frac{\partial Z}{\partial W} = \frac{A-Y}{A(1-A)} * A(1-A) * X = (A-Y)X = np.dot(X.T,\ A-Y)$
      - $db = \frac{\partial C}{\partial b} = \frac{\partial C}{\partial A}\frac{\partial A}{\partial Z}\frac{\partial Z}{\partial b} = A - Y = np.sum(A-Y)$
    - Update parameter: (i) $w\ =\ w -\ lr * dW$ (ii) $b\ =\ b -\ lr * dB$

(2) Naïve Bayes classifier: Uses Bayes theorem to classify data points. First, compute prior and likelihood for the classes, and then assign a data point to the class whose posterior probability is the highest; e.g., to determine if D_i falls into class θ:

- Bayes theorem: $P(\theta|D) = \frac{L(\theta|D)P(\theta)}{P(D)}$ → a way to update probability estimate as more evidence is available.
- Naïve independence assumption: Features are independent given the class, i.e., identity covariance matrix for all classes. This simplifies the likelihood computation: $L(\theta|\mathbf{D}) = P(\mathbf{D}|\theta) = \prod_{i=1}^{n} P(D_i|\theta)$
- Naïve Bayes classifier: $P(\theta|\mathbf{D}) = \frac{P(\theta)\prod P(D_i|\theta)}{P(\mathbf{D})} \propto P(\theta)\prod_{i=1}^{n} P(D_i|\theta)$
- Predicted class: $\hat{\theta} = \underset{Y}{\mathrm{argmax}}[P(\theta)\prod_{i=1}^{n} P(D_i|\theta)]$
- Types of Naïve Bayes: Gaussian: $P(D_i|\theta)$ is computed using Gaussian distribution and is used for features that follow normal distribution. Bernoulli: $P(D_i|\theta)$ is computed using Binomial distribution and is used for binary features. For text classification, use either Binomial (one-hot-encoding) or Multinomial (word count, TF-IDF) distributions.

(3) Maximum margin classifier: SVM (concepts: hyperplane/decision boundary, margins, support vectors, kernel trick)


ζ = 0
$w^Tx_i+b > +1$
positive margin: $w^Tx_i+b = +1$
$w^Tx_i+b = 1-ζ_i$
MARGIN
ζ > 0
decision boundary: $w^Tx_i+b = 0$
$w^Tx_i+b = -(1-ζ_i)$
negative margin: $w^Tx_i+b = -1$
$w^Tx_i+b < -1$
ζ = 0

- Class labels: y= $\{+1, -1\}$
- Margins: $w^TX + b \geq +1$, and, $w^TX + b \leq -1$. Multiply each side by y, we get a single equation to represent the margin: $y(w^TX + b) \geq 1$
- Distance between two margins: $d = \frac{2}{\|w\|}$. So, for maximum margin classification: $\max d \approx \min w \approx \min \frac{1}{2}\|w\|^2$

- Hard margin: Minimize $L = \frac{1}{2}\|w\|^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w}$ subject to $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$ ← this is L in primal form. Now we convert it to dual form. $\mathbf{x}_i$ is the i^{th} sample that includes all n features that's why we use transpose of w.
- Lagrange found that minimum of f(x) is found under constraint g(x)=0 when their gradients point in the same direction, i.e., $\nabla f(x) = \alpha\nabla g(x)$ or $\nabla f(x) - \alpha\nabla g(x) = 0$. Converting loss primal into dual form using Lagrange multiplier:

$$L = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum\alpha_i\{y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1\}, \qquad \frac{\partial L}{\partial w} = \mathbf{w} - \sum\alpha_i y_i\mathbf{x}_i = 0 \rightarrow \mathbf{w} = \sum\alpha_i y_i\mathbf{x}_i, \qquad \text{and } \frac{\partial L}{\partial b} = -\sum\alpha_i y_i = 0$$

$$\text{So, } L = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum\alpha_i\{y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1\} = \frac{1}{2}\mathbf{w}^T\sum\alpha_i y_i\mathbf{x}_i - \mathbf{w}^T\sum\alpha_i y_i\mathbf{x}_i - \sum\alpha_i y_i b + \sum\alpha_i = \sum\alpha_i - \frac{1}{2}\mathbf{w}^T\sum\alpha_i y_i\mathbf{x}_i$$

$$= \sum\alpha_i - \frac{1}{2}\sum\alpha_i y_i\mathbf{x}_i\sum\alpha_j y_j\mathbf{x}_j \Rightarrow L = \sum\alpha_i - \frac{1}{2}\sum\sum\alpha_i\alpha_j y_i y_j(\mathbf{x}_i.\mathbf{x}_j) \leftarrow \text{this is L in dual form.}$$

  - $\mathbf{w} = \sum\alpha_i y_i\mathbf{x}_i$, i.e., weight is a linear combination of some inputs
  - $L = \sum\alpha_i - \frac{1}{2}\sum\sum\alpha_i\alpha_j y_i y_j(\mathbf{x}_i.\mathbf{x}_j)$, i.e., optimization depends on the dot product of the inputs—kernel trick—maps the original into a higher-dimensional space where a linear separator can be found. Common kernels: Linear: $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i.\mathbf{x}_j$; Polynomial: $k(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i.\mathbf{x}_j)^d$; RBF: $k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$
- Soft margin: Minimize $\frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum\zeta_i$ subject to $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \zeta_i$
  - $\zeta_i \geq 0$ is slack variable for i^{th} sample, represent distance from margins; allow misclassification with $\zeta_i > 1$ when positive margin $y_i(\mathbf{w}^T\mathbf{x}_i + b) = 1 - \zeta_i$ falls below the decision boundary, vice versa for negatives.
  - $\zeta_i = \begin{cases} 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b) & \text{if } y_i \text{ is inside MARGIN, } y_i(\mathbf{w}^T\mathbf{x}_i + b) < 1 \\ 0 & \text{if } y_i \text{ is outside MARGIN, } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \end{cases} = \underbrace{\max\left(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)}_{\text{hinge loss}}$
  - Optimization: $\frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum\zeta_i = \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L2 regularizer}} + C\sum\underbrace{\max\left(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)}_{\text{hinge loss}}$
  - Same math for soft margin for w and L, but $0 < \alpha_i < C$.

(4) Trees: decision trees

- Which feature to split? Split based on the feature that gives minimum Gini impurity and maximum information gain.

$$GI = 1 - \sum_i p_i^2, \qquad IG = -\sum_i p_i \log p_i$$

  - Example: Play (yes/no) golf if the wind is high/low?
    - High (yes: 2; no: 3) → $GI = 1 - P(yes)^2 - P(no)^2 = 1 - \left(\frac{2}{5}\right)^2 - \left(\frac{3}{5}\right)^2 = 1 - \frac{4}{25} - \frac{9}{25} = \frac{12}{25}$
    - Low (yes: 6, no: 3) → $GI = 1 - P(yes)^2 - P(no)^2 = 1 - \left(\frac{6}{9}\right)^2 - \left(\frac{3}{9}\right)^2 = 1 - \frac{36}{81} - \frac{9}{81} = \frac{36}{81}$
    - GI for wind: 12/25 * (5/(5+9)) + 36/81 * (9/(5+9))
- Early stopping criteria (hyper-parameter optimization):
  - Max depth, max leaf nodes, minimum #sample to split a node, max #features to split, GI/IG tolerance etc.
  - Pruning: $\text{Cost} = \text{Loss} + \gamma T + \frac{1}{2}\lambda\sum_{i=1}^{T}\|w_i\|^2$, Loss: MSE , or log loss, T: number leaves, w_i: prediction score of i^{th} leaf

(5) Ensembles

- Bagging: Use bootstrapped observations (i.e., with replacement) to create a tree (split on 'best' features); create n-trees by repeating; train all trees in parallel.
    - Parallel training, computationally less expensive, easier to scale; Preferred when the model is complex, and we are concerned about overfitting problem.
    - Uses fully grown trees (individual tree has low bias & high variance) -> tries to reduce variance by adding predictors without affecting the bias (theoretically); for P predictors mu=mu and var=var/P, i.e., the mean of aggregated predictions remains same as the mean of individual models, while the variance of aggregated predictions is reduced by a factor of P, the number of models.
        - Given $\mathrm{m_1, m_2, \ldots, m_p}$ as predictions from p different models, the aggregated prediction x is the average of these predictions: $\mathrm{m} = \frac{\mathrm{m_1+m_2+\cdots+m_p}}{\mathrm{p}}$
        - $\mathrm{mean(m)} = \mathrm{E[m]} = \frac{\mathrm{E[m_1]+E[m_2]\ldots+E[m_p]}}{\mathrm{P}} = \mathrm{P} * \frac{\mu}{\mathrm{P}} = \mu$
        - $\mathrm{var(m)} = \mathrm{E[(m-\mu)^2]} = \mathrm{E}\left[\left(\frac{\mathrm{m_1+m_2\ldots+m_p}}{\mathrm{P}} - \mu\right)^2\right] = \frac{1}{\mathrm{P^2}} * \mathrm{E}\left[\left((\mathrm{m_1}-\mu) + (\mathrm{m_2}-\mu)\ldots + (\mathrm{m_p}-\mu)\right)^2\right] \rightarrow$ apply iid assumption $\rightarrow \mathrm{var(m)} = \frac{1}{\mathrm{P^2}} * \mathrm{E}\left[(\mathrm{m_1}-\mu)^2 + (\mathrm{m_2}-\mu)^2 \ldots + (\mathrm{m_p}-\mu)^2\right] = \frac{1}{\mathrm{P^2}} * \mathrm{P} * \sigma^2 = \sigma^2/\mathrm{P}$
    - Two commonly used variants of bagging methods:
        - Random forest (RF): Use bootstrapped observations and randomly select several features and split on the 'best' feature (from the selected ones); repeat for n-trees.
        - Extremely RF: Bootstrapped observations, select some random features, split a random feature.
- Boosting: Train the first model, increase the weights to the observations that are incorrectly predicted by the first model, and then train the second model, and so on.
    - Sequential training, computationally expensive, hard to scale; Preferred when the model is simple, and we are concerned about underfitting problem.
    - Uses shallow trees (individual tree has high bias & low variance) -> tries to reduce bias by adding predictors into the ensemble without affecting the variance (theoretically); variance increases but can be controlled by limiting number of weak learners, using pruning, regularization. In XGBoost:

$$\mathrm{Cost} = \mathrm{Loss} + \gamma\mathrm{T} + \frac{1}{2}\lambda\sum_{i=1}^{T} \|\mathrm{w_i}\|^2, \mathrm{Loss{:}\ MSE\ , or\ log\ loss, T{:}\ number\ leaves, w_i{:}\ prediction\ score\ of\ i^{th}\ leaf}$$

    - Two commonly used boosting methods:
        - Gradient boosting
            - Initialize the prediction with a constant, typically with the mean of the output.
            - For estimator i = 1, 2, …, P
                - If i=1: Train estimator i with the original data
                - Else: Train estimator i with the residuals from combined estimators [1, i-1]; "<u>residuals", so used in regression</u>.
        - AdaBoost:
            - Start with equal weights (α) to all observations, i.e. $\alpha_i = 1/n$
            - For estimator i = 1, 2, …, P
                - Train estimator i and compute its coefficient (using weighted error)
                - Re-compute the weights of the observations, i.e., increase the weights to misclassified observations; "<u>misclassification", so used in classification</u>.
- <u>Stacking</u>: Train k estimators and use the outputs of the k estimator as the input to another estimator.

CLUSTERING

(1) K-means

- Uses a partitioning algorithm; Needs to predefine the number of clusters; Hard assignment.
- Assumption: Clusters are spherical and isotropic (uniform in all directions), and all clusters have same variance.
- Method: Initialize the center (mean) of the clusters. Compute the distance of each observation from the clusters and assign the observation to its nearest cluster. Update the means of the cluster and repeat until convergence.
- May suffer from local minima problem
- Determine the number of clusters: Prior knowledge, elbow method.

(2) Gaussian mixture model

- Uses a probabilistic algorithm; Needs to predefine the number of clusters; Soft assignment.
- Assumption: Data can be interpreted as a mixture of Gaussian distributions
- Method: Initialize center (mean) and shape (variance) and update them using EM algorithm
    - Prior: $\pi_c = \frac{n_c}{n}$, n_c: number of data points in cluster c, n: total number of datapoints in the dataset.
    - E-step: compute soft probability of i^{th} sample x_i being in cluster c: $r_{ic} = \frac{\pi_c N(x_i;\mu_c,\Sigma_c)}{\sum \pi_k N(x_i;\mu_k,\Sigma_k)} \approx P(c|D) = \frac{P(c)P(D|c)}{P(D)}$
    - M-step: Update π_c, μ_c and Σ_c: $\pi_c = \frac{\pi_c}{\sum r_{ic}}$, $\mu_c = \frac{\sum r_{ic} x_i}{\sum r_{ic}}$ and $\Sigma_c = \frac{\sum r_{ic}(x_i-\mu_c)^T(x_i-\mu_c)}{\sum r_{ic}}$

(3) DBSCAN: Density-Based Spatial Clustering Application with Noise

- Uses a density-based algorithm; no need to predefine the number of clusters; arbitrary shape of clusters.
- Grouping points together in high-density regions and marking points as noise in low-density regions. Core points (having a minimum number of other points within a given radius ϵ), border points (fewer neighbors but close to a core point), and noise (points not part of any cluster).
- Method: Start with a point and check if it's a core. If so, form a cluster with all points within ϵ-distance. For each point in the cluster, check if they are core. If they are core, expand the original cluster with their neighbors. If they are not core, mark them as border. Mark any left-out points as noise. Example with points: A, B, C, D, E, F. Cluster parameters: min-points=2 and $\epsilon = 1.5$. Point : neighbors = A: b; B: a, c; C: b, d; D: c, E: f, F: e. → Start with A, not a core due to only 1 neighbor → Move to B, a core point, initiating a cluster with B, A, C → Expand cluster from each point in it → A not a core, mark it as border → C is a core, expand the cluster to B, A, C, D → Expand from D, which is not a core, mark it as border → Continue with next unvisited points → E and F, each with only one neighbor and unable to form a core, are marked as noise.

(4) Hierarchical clustering

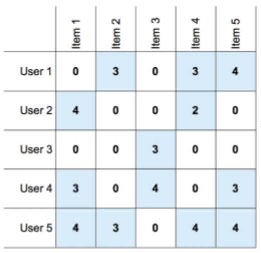
- Uses agglomerative (bottom-up) vs. divisive (top-down) algorithms; No need to predefine the number of clusters.
- Assumption: Data structures maintain a hierarchy.
- Distance/Linkage metrics: Ward's, simple (minimum), complete (maximum), average
- Bottom-up method: Start with each data point as a cluster. Then merge two clusters based on the distances. Repeat the process until all data points form one cluster.

(5) Cluster validation

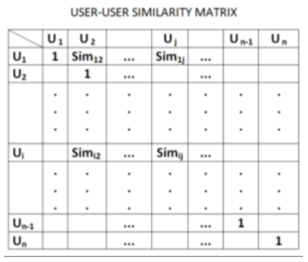
- Human evaluation > supervised evaluation > index-based evaluation
- Supervised evaluation: Shows the similarity between true labels and cluster labels (rand index).
- Index: Minimize the variance within a cluster and maximize the separation between the clusters (Dunn index).

Recommender systems

- Recommendation types
  - Content-based (focuses on item attributes)
    - Summary statistics: Recommend popular items, recommend items with average prices, etc.
    - Clustering and kNN and then recommend k products (using distance metrics (Cosine, Euclidean) or document representations (TF-IDF)
  - Collaborative Filtering (relies on item-user similarities)
    - Learn feature vectors for the products and for the users simultaneously, which are used to recommend specific products to specific users.

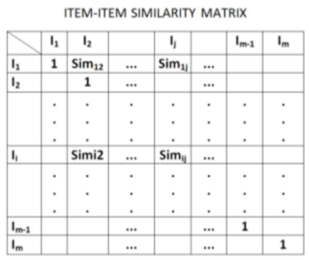


	Item 1	Item 2	Item 3	Item 4	Item 5
User 1	0	3	0	3	4
User 2	4	0	0	2	0
User 3	0	0	3	0	0
User 4	3	0	4	0	3
User 5	4	3	0	4	4



USER-USER SIMILARITY MATRIX

	U_1	U_2		U_j		U_{n-1}	U_n
U_1	1	Sim_{12}	...	Sim_{1j}	...		
U_2		1	...		...		
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
U_i		Sim_{i2}	...	Sim_{ij}	...		
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
U_{n-1}			...		...	1	
U_n			...		...		1



ITEM-ITEM SIMILARITY MATRIX

	I_1	I_2		I_j		I_{m-1}	I_m
I_1	1	Sim_{12}	...	Sim_{1j}	...		
I_2		1	...		...		
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
I_i		Simi2	...	Sim_{ij}	...		
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
I_{m-1}			...		...	1	
I_m			...		...		1

    - User-user-based collaborative filtering
      - Compute user-user similarity matrix; pick the most similar users (similar to target user); get the items that those users liked; and recommend those to the target user.
    - Item-item-based collaborative filtering
      - Compute item-item similarity matrix; get the most similar items. E.g., user5 already liked items 1, 4, and 5, so find out the items similar to 1, 4, and 5, and recommend the most common ones from the three sets.
    - Matrix Factorization: K = U * V => user-item matrix = user matrix * item matrix
      - K (m x n) = U (m x d) * V (d * n) with d features for users and items
      - Initialize U and V; then update U and V iteratively so that $\mathrm{UV} \rightarrow \mathrm{K}$.
      - Optimize the number of features (d), learning rate (α), and regularization strength (λ).

$$\mathrm{L} = \frac{1}{2}\sum_{\mathrm{i,j}}\left(\mathrm{r_{ij}} - \mathrm{u_i^T v_j}\right)^2 + \frac{\lambda}{2}\left(\sum_{\mathrm{i}}\|\mathrm{u_i}\|^2 + \left\|\mathrm{v_j}\right\|^2\right), \qquad \mathrm{u_i} = \mathrm{u_i} - \alpha\frac{\partial \mathrm{L}}{\mathrm{du_i}}$$

  - Hybrid (combination of content-based and collaborative filtering)
- Evaluation: Measuring success of recommender systems
  - Offline: MAE, MSE, Precision, Recall, NDCG, TPR, FPR, ROC-AUC
  - Online: Click Through Rate **->** Adoption and Conversion **->** Sales and Revenue
- Challenges
  - Cold start problem: no or limited data available for a new user or item -> use content-based recommendation to minimize this problem.
  - Long-tail problem: many items have few or no ratings -> skewed distribution of recommendation towards popular items -> items in the long tail of distribution are overlooked -> solve using matrix factorization.
- Building a recommendation system from scratch
  - Problem/Scope -> data collection -> feature engineering -> algorithm selection -> training/validating -> deploying -> monitoring performance -> CD/CI
  - Scaling: Layered modeling (clustering, matrix factorization, deep learning) and distributed computing.

LINEAR ALGEBRA and DIMENSIONALITY REDUCTION

(1) Matrix (Fundamentals: Transpose, inverse, identity, diagonal, triangular, symmetric, trace)

- Linearly independent matrix: No columns can be written as a linear combination of the others. Columns of a matrix are linearly independent if there exists only a trivial solution to Ax = 0, i.e., x = 0 vector.
  - Rank: Number of independent columns or rows
  - Nullity: Null space is the set of all vectors x for which Ax = 0; for full-rank matrix, null space is $\underline{x}$=0
  - Rank-Nullity Theorem: Rank(A) + Nullity(A) = Number of columns in A
- Orthogonal/orthonormal matrices: Rows and columns are orthogonal unit vectors, i.e., $AA^T = A^TA = I$.
  - Dot product between any row and any column is zero (orthogonality)
  - Dot product of any row (or column) with itself is one (orthonormality)
  - Gram-Schimdt method: Turns a set of linearly independent vectors into a set of orthogonal vectors.
- Norm: Measures size/weight/intensity of matrix in terms of the magnitudes of elements, e.g., Frobenius (L2) norm.
- Jacobian: First derivative of a multivariate function → used for system analysis, e.g., how small changes in inputs affect output); also used in optimization.

(2) Eigenvectors and eigenvalues (of square matrix)

- $\mathbf{Av = \lambda v}$ **→ the vectors multiplied by A results in the same vector with a difference in scaler magnitude are called as the eigenvectors**. Eigenvectors represent the direction of linear transformation of a matrix, and eigenvalues represent the strength of the vectors in their directions.
- Eigenvalue decomposition theory states that any real, symmetric matrix ($\Sigma = \Sigma^T$) can be represented as $\Sigma = Q\Lambda Q^T$, where Q is the orthogonal matrix, whose columns are eigenvectors; therefore, **all eigenvectors are orthogonal to each other**. Λ is a diagonal matrix whose diagonal elements are the eigenvalues.
- **Eigenvectors of a matrix (e.g., matrix = covariance matrix of data) give us the directions of maximum variance, which is PCA**: $\lambda v = \Sigma v \rightarrow v^T\lambda v = v^T\Sigma v \rightarrow \lambda v^T v = v^T\Sigma v \leftarrow \text{variance of data when projected onto v direction.}$

$$\text{i.e.}, v^T\Sigma v = v^T\frac{1}{n}\sum_i (x_i-\mu)^T(x_i-\mu)\,v = \frac{1}{n}\sum_i v^T(x_i-\mu)^T(x_i-\mu)v = \frac{1}{n}\sum_i [(x_i-\mu)v]^T[(x_i-\mu)v] = \frac{1}{n}\sum_i p_i^Tp_i = \sigma_p^2$$

  We want to find a direction that maximizes the variance $v^T\Sigma v$. Or equivalently maximizes λv^Tv. It is maximum when $v^Tv = 1$, which leaves $\lambda = v^T\Sigma v$, i.e., λ is the maximum variance of data matrix Σ when projected onto v direction.

(3) PCA

- **By projecting data onto these eigenvectors, PCA achieves dimensionality reduction while retaining the most significant variance features of the original data.**
- Assumption for PCA: Data follows a Gaussian distribution
- Eigenvectors are orthogonal, so no collinearity between the dimensions. PCA is often implemented using SVD.

(4) SVD

- $\mathbf{A = U\,S\,V^T}$ **→ Principal Components (PCs) in PCA correspond to the columns of U, and singular values or diagonal values of S give the amount of variance captured by each PC.**
- Diagonal values of S = Singular values of A = sqrt(eigenvalues of AA^T or A^TA) or $\sigma = \sqrt{\lambda}$
- Columns of U = Eigenvectors of AA^T (covariance matrix of A in its row/observation space) = Left singular vectors. Form an orthonormal basis of column space of A; Rows of A are linear combination o left singular vectors.
- Columns of V = Eigenvectors of A^TA (covariance matrix of A in its col/feature space) = Right singular vectors. Forms an orthonormal basis of row space of A; Columns of A are linear combination of right singular vectors → **Columns of V are used as PCs in PCA**.
- Reduced dimension: $A_{mxd} = U_{mxd}S_{dxd}$ and data approximation: $\widehat{A}_{mxn} = U_{mxd}S_{dxd}V_{dxn}^T$

(5) ICA: Data sources are independent and have non-Gaussian distributions; Tries to find and separate different sources.

PROBABILITY and STATISTICS

- Difference between probability and likelihood
  - Probability: Measures chance of event given the known parameters: P(data | parameters)
    - P(weight > 60kg | mu=0, sigma=1) → think of area under the distribution function!
  - Likelihood: Measures the plausibility of parameters given the observed data: L(parameters | data)
    - L(mu=0, sigma=1 | weight > 60kg) → think for fitting the data to a distribution!
- Independent events: Probability of occurring an event does not depend on the other events.
  - P(A or B) = P(A) + P(B) – P(A and B) → for two events
    - P(A and B) = P(A) * P(B) → for independent events
    - P(A and B) = P(A) * P(B|A) = P(B) * P(A|B) → for dependent events
    - P(A and B) = 0 → for mutually exclusive events
- Conditional Probability: Probability of an event occurring given that another event has already been occurred P(A|B)
- Bayes' Theorem: It provides a way to update our knowledge or beliefs (probability) based on prior evidence as: P(A|B) = P(B|A) * P(A) / P(B)
- Random variables: outcome of random phenomena → expressed as binomial, Poisson, and normal distributions.

Distribution	Definition	Mean and Variance	Use Cases
Binomial	Probability of getting exactly k successes in n trials: $$P(X=k)=\binom{n}{k}p^k(1-p)^{n-k}$$	$\mu = np$, $\sigma^2 = npq$	Predicting the number of defective items in batch of products
Poisson	Probability of observing k events in an interval: $$P(X=k)=\frac{\lambda^k e^{-\lambda}}{k!}$$	$\mu = \lambda$, $\sigma^2 = \lambda$	Counting something in an interval, e.g. number of error in a page
Normal	Probability density function: $$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$	$\mu = \mu$, $\sigma^2 = \sigma^2$	Modeling heights or weights of population

- Sampling methods (Random, Stratified random, cluster random, systematic)
- Statistical measures
  - Central tendency (mean, median, mode) and variability (variance, standard deviation, range, IQR)
  - Asymmetry (skewness) → right/positive skewed → mode < median < mean.
  - Peakness (kurtosis) → k=0 normal; k=3 pointy; k = –0.6 semi-circular; k = –1.2 square.
- Central Limit Theorem: Mean of means follow a normal distribution with μ = population mean, σ = population σ / √n.
- Law of Large Numbers: For large sample size, the sample statistics tend to population/expected statistics.
- Hypothesis testing: Statistical methods of evaluating two propositions (null and alternative hypothesis)
  - A/B testing: Test two versions by measuring a metric from two randomly selected groups.
- P-value and confidence interval
  - P = Probability of getting a statistic as extreme as or more extreme than the observed one given the null hypothesis is true, i.e., the likelihood of getting a data by chance given the null hypothesis is true.
  - 95% CI = If we repeat the same experiment and compute a new CI every time, then the true population statistic is expected to fall the CI for 95% cases.

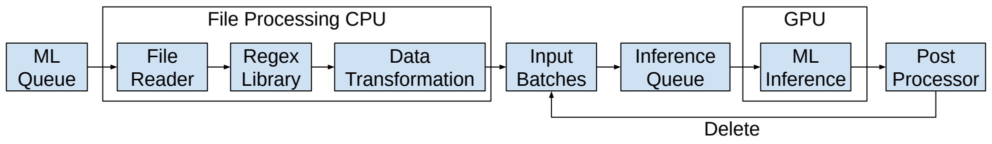
- Statistical Power: The power of a statistical test is the probability that the test will reject null hypothesis when the alternative hypothesis is true. It's denoted as $1 - \beta$, where β is the probability of making a Type II error (failing to reject null hypothesis when alternative hypothesis is true).
    - Power Analysis: Method of calculating required sample size to achieve a desired significance level ($\alpha =$ the probability of making a Type I error) and effect size (magnitude of difference).
    - There's a tradeoff between α and β → increasing α decreases β, therefore increases statistical power.
    - α (Type I error) is associated with FP that impacts precision, while β (Type II error) is associated with FN that impacts recall).
- Choice of statistical tests

IN\OUT	Categorical	Continuous
Categorical	Chi-Square, ANCOVA	T-tests (smaller n), Z-test (larger n>30), ANOVA
Continuous	Logistic Regression	Regression

    - 1-sample and 2-sample tests (t-test, z-test), n-sample tests (ANOVA, ANCOVA), association tests (correlation between two qualitative (chi-square) or quantitative (regression) variables).
- Parametric and non-parametric methods
    - Parametric: Assume data follow a distribution (used to make inference about population parameters)
    - Non-parametric: No assumption

Parametric Tests	**Equivalent non-parametric tests**
T-tests	Independent: Mann-Whitney-U Dependent: Wilcoxon signed rank
ANOVA	1-way: Kruskal-Wallis 2-way: Friedman
Chi-Square	Fisher's exact test
Correlation	Spearman's rank correlation

Data detection with ML



- NLP-based DL: design, training, fine-tuning, deploying. Precision 35% → 60%.
    - CharCNN (replace each char in the string by its index from 69 alphabets; make its length 160 by padding 0s if string is shorter; represent each index by an embedding of size 32, which gives 160x32 matrix representation of the input text; apply convolution with 256 filters each of size 7x32 and max pooling with filter size of 3x1); Size: input (160x1) → embedding (160x32) → convolution (160x256) → maxpool (80x256)
    - 6 Conv layers (256 features, 7/3 kernel, 3/0 pool); 3 linear layers (512, 512, 1)
- Golden data: Create labels using LLM/GenAI, use that to train DL. Precision 60% → 72%.
    - Design experiment → collect → (1) send to human; not scalable (2) generate labels, 95% accuracy (used fine-tuning and prompt-tuning).
- Research: model reduction for faster inference with limited resources.
    - Pruning
        - Strategy: Drop layers based on weight magnitude vs drop layers iteratively
        - Process: Prune selected layers and fine-tune the remaining
    - Quantization
        - Strategy: From 32 bits to 16 or 8 bits
        - Process: (I) post-training quantization and (II) Quantization-aware training
    - Weight SVD
        - $y_{mx1} = W_{mxn}x_{nx1} = U_{mxk}S_{kxk}V_{kxn}^T x_{nx1}$, where m = number of out neurons/features, n = number of input neurons/features ($W_Q, W_K, W_V, W_O, W_{ff1}, W_{ff2}, \gamma_{attn}, \beta_{attn}, \gamma_{ff}, \beta_{ff}$)
    - Sparse Attention
        - Use sparse attention weights to reduce computations
    - Combined
        - Sequential: Quantization followed by Pruning or vice versa
        - Simultaneous: Quantization-aware training with randomly selected layers pruned
    - Memory = param + activation + gradient + buffer = 10GB + 3*10GB + 3*10GB + 70GB*10% = 77GB
        - Params: 2.5B each of 4 bytes (FP32)
        - Training takes 1 hour with 4 H100 in 100k steps → A100: 80GB RAM, 1000 TFLOPs/sec
        - Inference: 7ms for a query with ~15 words vs. 16ms with original model.
            - ~1 hour for half-million queries vs. 20min with charCNN, but at nearly same cost.

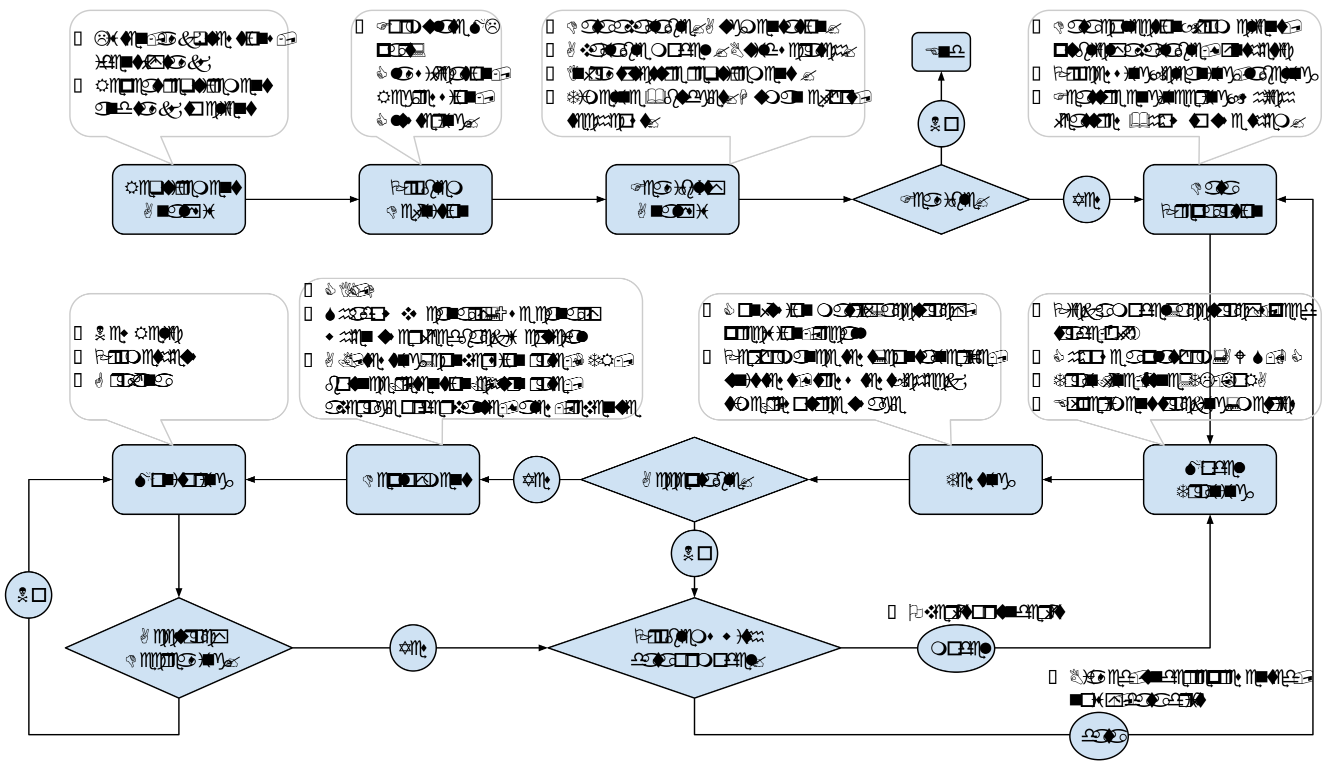
Document Recommendation

- 3 steps: Graph, TF-IDF, and Transformer (BERT-base)
- Transformer BERT approach details:
    - **Data preparation**
        - A-A*: Similar documents. A* is prepared by replacing words in A by their synonyms.
        - A-B: Dissimilar documents. Use usage graph to find dissimilar docs with distance > 3.
    - **Data table:**

Pair	Label (y)
A-A*	0
A-B	1

    - **Contrastive loss**
        - $L = (1-y) * \|x_i - x_j\|_2^2 + y * \max\left(0, m - \|x_i - x_j\|_2^2\right)$
        - $y = 0 \Rightarrow L = \|x_i - x_j\|_2^2 \Rightarrow \text{for similar docs, larger euclidean distance is penalized.}$
        - $y = 1 \Rightarrow L = \max\left(0, m - \|x_i - x_j\|_2^2\right) \Rightarrow \text{for dissimilar docs, euclidean distance} < m \text{ is penalized.}$
        - m too large => dissimilar docs fall farther apart. Distance < m will be penalized, so too large value of m might be good for two docs that are fully different, but models won't learn to distinguish docs with similarity distance less than m.
    - **Training: With LoRA (Low Rank Adoption)**
        - $W = W + W_r = W + AB,\ W^*, W, W_r \in \mathbb{R}^{m\times n}; A \in \mathbb{R}^{m\times r}, B \in \mathbb{R}^{r\times n}; r \ll m, n$
    - **Evaluation**
        - Precision: Proportion of likes improves from 60% to 80%, i.e., 8 out of 10 recommended documents were liked by the users, while recall remains the same at 90% for TF-IDF vs. BERT models.
    - **Candidate selection model**
        - Select candidate documents from usage graph with distance <= 2. If the number of candidates > 500, apply TF-IDF cosine similarity to filter out the candidates.
    - 5 people (1 MLE: design, data sources, format, model training, deployment; 3 DS: data prep, analysis, build graph, build data table for bert, model building (jaccard, tf-idf, bert); 1 SWE: deployment).

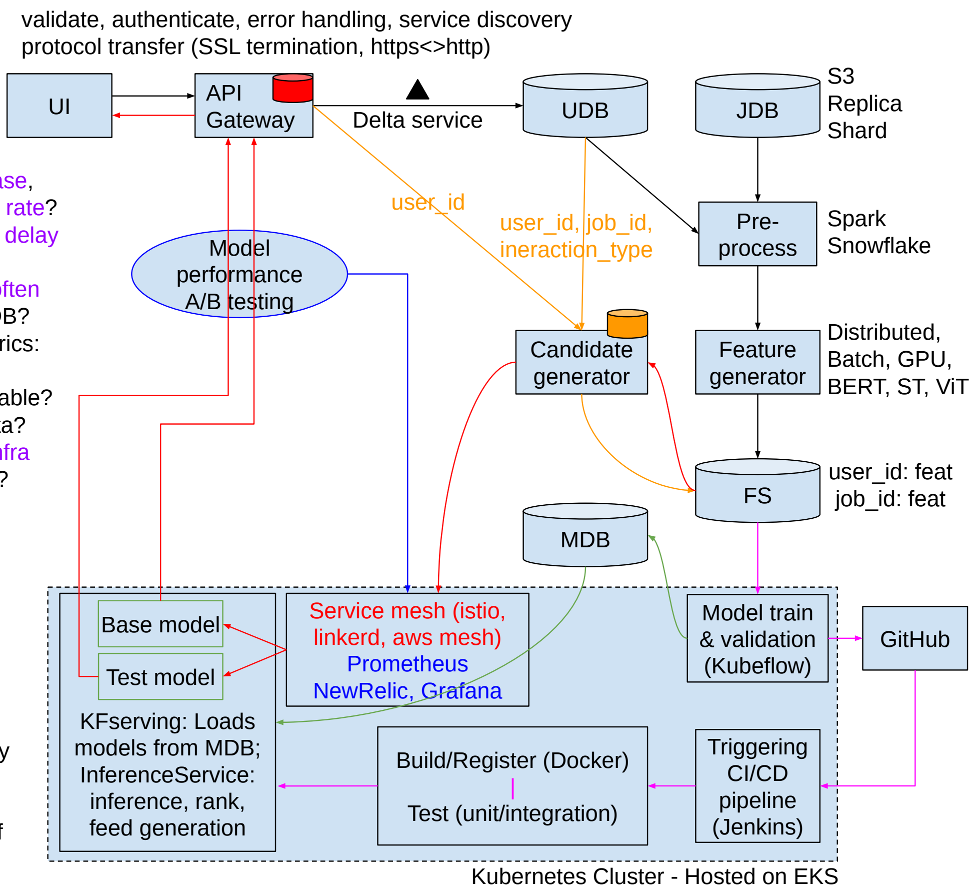
ML System Design: E2E ML Workflow



- Training
    - Build model class (includes three building blocks: position encoding, attention mechanisms, feedforward)
    - Data: input-target pairs and their tokens
    - Model, loss function, optimizer
    - Train and validate: Bach feed, training/validation loss per epoch

Problem Name	**Best ML Models**	**Cost, Optimization, Evaluation**
Recommendation (LinkedIn job, Netflix movie, YouTube video, E-commerce product, Events, News feed) (A/B tests: t-test with equal var; Welch's t-test if group sizes vary largely)	TF-IDF, Collaborative Filtering, Matrix Factorization, BERT, ST Pairwise Loss is for Ranking Cross-Entropy is for Classification	• Personalized? User-X interaction data? • Pairwise Loss=max(0, 1 – (sim$^+$ – sim$^-$)) Data Table: (uid, +/-pair, +sim, -sim) • Local tests: Precision@k, NDCG@k
Classification (Ads click, Article tagging, Harmful content detection, Transaction fraud, Server logs anomaly)	Logistic Regression, Gradient Boosting, Random Forests, Isolation Forests (unsupervised), LSTM, CNN, BERT	• Number of tags? harmful/anomaly/fraud? • Cross-Entropy • Accuracy • Precision, Recall, F1-score, AUC-ROC
Object Detection/Segmentation (Face, Pedestrians, Facemask)	U-Net, YOLO, ViT (classification), Swin Transformer (detection)	• Partial visibility or occlusion? • Cross-Entropy, Dice Coeff, IOU • Precision, Recall, F1-score, mAP
Regression Prediction (Traffic pattern for GPS app, Stock price)	ARIMA, LSTM, Prophet	• Time horizon? Factors (weather, event)? • MSE, MAE, RMSE

ML System Design: Deployment Infrastructure and Operational Pipelines


validate, authenticate, error handling, service discovery
protocol transfer (SSL termination, https<>http)
UI
API Gateway
Delta service
UDB
JDB
S3
Replica
Shard
user_id
user_id, job_id, ineraction_type
Pre-process
Spark
Snowflake
Model performance A/B testing
Candidate generator
Feature generator
Distributed, Batch, GPU, BERT, ST, ViT
FS
user_id: feat
job_id: feat
MDB
Base model
Test model
Service mesh (istio, linkerd, aws mesh)
Prometheus
NewRelic, Grafana
Model train & validation (Kubeflow)
GitHub
KFserving: Loads models from MDB; InferenceService: inference, rank, feed generation
Build/Register (Docker)
Test (unit/integration)
Triggering CI/CD pipeline (Jenkins)
Kubernetes Cluster - Hosted on EKS

Clarification Questions

1. Scale: Size of user base, DB, QPS, and growth rate?
2. Latency: Real-time or delay acceptable?
3. Scale/Latency: How often new items added to DB?
4. Model evaluation metrics: Business objective?
5. Data: Train data available? What feature/metadata?
6. Focus: Algorithm or infra development, or both?

Scalability, Availability

1. Microservices
2. Distributed services
3. Caching
4. Load balancing
5. Logging & Monitoring
6. Rate limiting
7. Replication/Sharding
8. Complexity vs Latency
9. Cold start problem
10. Privacy & Security
11. Bias-variance tradeoff

- Data
  - Exploration and handling missing data and outliers
    - Missing data: Imputation, Regression, SVD
    - Outliers: data point >= 2 * z-score/standard deviation, or use anomaly detection algorithms
  - Feature engineering/generation (embeddings, transformation, normalization, scaling)
  - Train/test split: 80/20, Cross-validation for limited amount of data
- Model Deployment
  - Train and validate model (using in-house tools and workflows, or within kubeflow) --> save the model in .onnx format and upload to artifactory --> push changes to github with yaml configuration file --> jenkins runs builds, tests, and deploy ServiceInference (kubectl apply -f file.yaml) --> KFServing is now operational, handles incoming inference requests, and scales based on the traffic.
  - Now, ServiceInference is accessible via a specific URL provided by Kubernetes cluster's ingress or load balancer. To send inference request, create a script that runs in a regular basis. The script contain the URL and link to dataset that is to make inference for. YAML file contains storageUri (model path), predictor (torch), compute resources, scaling parameters (pods), deployment command.
  - CI/CD pipeline
    - CI (change, push, build, test); CD (canary deployment or whole system deployment).
    - **GitHub Actions** (hosted by GitHub, suitable for simple workflows); **Jenkins** (self-hosted, suitable for more complex workflow since it is more configurable).

Kubeflow (open-source, customizable, uses Kubernetes infra); **Sagemaker** (AWS hosted); **MLflow** (open-source, less developed); **Airflow** (used for all workflows, not specialized for ML).

The goal of my project is to detect personally identifiable information (PII) such as SSNs and bank account numbers from text documents. The previous system solely relied on regex-based matching, which produced a lot of false positives and resulted in a low precision of about 35%. I used machine learning to solve this problem, and had taken three initiatives to improve the system step by step:

First, I built an NLP-based deep learning model, specifically a character-level CNN that involved designing, training, fine-tuning, and deploying the model in production. This model improved the precision from 35% to 60%.

Second was golden data collection. Our training data was noisy, and labeling them by humans was slow and not scalable. So, I used LLMs like Mistral 7B and fine-tuned them to generate more accurate labels at scale. Training the charCNN model with these generated labels improved the model's precision to 72%.

Third was focused on research around model compression. LLMs are generally good at detecting PII data but are too slow and resource-intensive for production. So, I researched model compression techniques like layer pruning, weight quantization, SVD, and sparse attention representation. This reduced the model size to one-third, cut inference time from 24ms to 7ms, while maintaining 87% precision.

General Understanding and Motivation
Q1: What motivated you to focus on model compression for your PII detection project?
A1: Better performance, slower inference, memory and resource-intensive therefore higher cost, not ideal at scale.

Q2: Why is model compression important for deploying machine learning models in production environments?
A2: To increase inference speed using limited resource and to reduce cost at scale.

Techniques and Implementation
Q3: Can you explain how layer pruning works and how you applied it in your project?
A3: Layer pruning (removing layers vs. making layer's weight spare using a threshold). I used a systematic way to selecting layers to keep/drop (more layers are only required to represent complex pattern in the data; starting from middle, keep/drop every other layers—encoder-decoder concept).

Q4: What is weight quantization, and how did it help reduce the model size and inference time?
A4: Reduce precision of floating-point numbers to lower bit-width integers such as 8-bit integers—reduces model size and accelerate computation. I used quantization-aware training.

Q5: How does Singular Value Decomposition (SVD) contribute to model compression, and how did you implement it?
A5: W = USVT—store U, S, and V at lower dimension—decreases computing loads and memory requirement.

Q6: Can you describe what sparse attention representation is and its role in your model compression efforts?
A6: Q, K — gives n x n — represents how each word is related with others—not all might be required—make USV of Q and K sparse and learn sparse USV representation of V.

Challenges and Solutions
Q7: What were the main challenges you faced during the model compression process?
A7: Reduced precision after pruning and quantization—addressed with fine-tuning—that introduced another challenge of resource—use systematic ways to prune.

Q8: How did you ensure that model accuracy was maintained after applying compression techniques?
A8: We employed a combination of quantization-aware training and incremental pruning, followed by fine-tuning. This process allowed us to adjust the model weights iteratively to recover any loss in accuracy. Regular validation against a held-out dataset ensured that the model's performance remained high.

Q9: Can you provide details on how you tested the compressed model to validate its performance?
A9: Validate using internal validation data, Monitor precision/recall, and approximate inference time and resource usage.

Results and Impact
Q10: What specific metrics did you use to measure the success of your model compression?
A10: Precision/recall, inference time, memory and resource usage.

Q11: How did the reduction in model size and inference time impact the overall system performance and cost?

A11:	Original LLM	Reduced LLM	charCNN
Precision	90%	87%	72%
Inference time	24ms	7ms (1 H100)	2ms
Cost	4*33k (to achieve 7ms)	33k	27k

Q12: Can you discuss any trade-offs you encountered between model size, inference time, and precision?
A12: Precision & speed vs. model size (strength of pruning), vs. SVD rank vs. quantization

Future Directions
Q13: What further optimizations or techniques would you consider to improve model efficiency in the future?
A13: Sparse attention representation: Q, K — gives n x n — represents how each word is related with others—not all might be required—make USV of Q and K sparse and learn sparse USV representation of V. And, combining model distillation with compression techniques

Q14: How do you see the field of model compression evolving, and what new methods are you excited about?
A14: zero-shot quantization and adaptive quantization; combining model distillation with compression techniques.

Technical Depth
Q15: Can you delve deeper into the mathematical foundation of SVD and how it aids in reducing computational complexity?
A15: SVD details

Q16: How did you handle potential overfitting or underfitting issues when applying these compression techniques?
A16: Monitor validation performance, early stopping during training

Behavioral Questions

- Tell yourself/experience/why be hired? → Passionate, qualified, ability to contribute, change my life.
- Strength → Diversified skills/ability to work across teams/mentoring.
- Weakness → Influence, Difficulty to use top skills in product development.
- Biggest accomplishment/e2e products → Meta recommendation
- Working with cross-functional teams → C1 LLMs/data science team, MLX teams, and privacy compliance teams.
- Failed and learned → Shell oil detection
- Conflict → Replacing scan by ML with VP; Meta recommendation // asset ownership at individual/team level
- Working in a fast-paced environment → C1 sprint-by-sprint, allocate times/resources, use management tools
- Establishing standard code review systems → (works, readable, maintainable) Template, minimum 2 approvals

Time Management
Tight deadline, multiple deadlines/prioritizing, missed deadline – Meta recommendation vs ownership prediction

Teamwork
Conflict, work with a difficult member, successful project worked on as a part of the team – ownership prediction
helped a team member to improve their performance – Jr SWE to MLE

Leadership/Initiative
Project took lead/initiative, motivate others to achieve a goal, mentor colleagues, delegating tasks – C1 project

Adaptability
Significant changes, sudden changes in priorities, had to learn something new quickly – model to infra development

Communication
Communicated complex issue/message, effective communication made a difference in project – replacing regex by ML
handle feedback giving and receiving --

Problem solving
Complex problem solved, major issue identified and solved, analyze information and make quick decision

Failure
Project that failed and what learned – Shell oil detection

Ethics
What motivates to works – helping people
went above and beyond job responsibilities/handle obstacles

Project Management
A project worked from start to finish, kept project on track – C1 project

Client
Deliver client needs, worked with a difficult client – Meta graph node quality

Cross-functional collaboration – DS, MLX, privacy, Card