Complete Mathematical Formulas in Machine Learning

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Foundational Mathematics

Basic Notation

- **Scalar**: Single value, denoted as x, y, a, b
- **Vector**: Column of values, denoted as **x**, **y** (bold)
- Matrix: 2D array, denoted as X, W (bold capital)
- **Tensor**: n-dimensional array

Summation and Product Notation

Summation:

$$\Sigma_{i=1}^{n} X_{i} = X_{1} + X_{2} + ... + X_{n}$$

Product:

Statistical Measures

Mean (Average)

Arithmetic Mean:

$$\mu = \bar{x} = (1/n) \times \Sigma_{i=1}^{n} x_{i}$$

- μ (mu) or \bar{x} represents the mean
- n is the number of observations
- x_i is the i-th observation

Variance

Population Variance:

$$\sigma^2 = (1/n) \times \Sigma_{i=1}^n (x_i - \mu)^2$$

Sample Variance (Bessel's correction):

$$S^2 = (1/(n-1)) \times \Sigma_{i=1}^n (x_i - \bar{x})^2$$

Standard Deviation

$$\sigma = \sqrt{(\sigma^2)}$$
 (population)
 $s = \sqrt{(s^2)}$ (sample)

Covariance

Between two variables X and Y:

$$Cov(X,Y) = (1/n) \times \Sigma_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y)$$

Correlation Coefficient

Pearson Correlation:

$$\rho(X,Y) = Cov(X,Y) / (\sigma_x \times \sigma_y)$$

• Range: [-1, 1]

- -1: perfect negative correlation
- 0: no linear correlation
- 1: perfect positive correlation

Standardization (Z-score)

$$z = (x - \mu) / \sigma$$

• Transforms data to have $\mu = 0$ and $\sigma = 1$

Linear Algebra in ML

Vector Operations

Dot Product (Inner Product):

$$a \cdot b = \sum_{i=1}^{n} a_i b_i = a_1 b_1 + a_2 b_2 + ... + a_n b_n$$

Vector Norm (Length):

- L1 Norm (Manhattan): $||x||_1 = \Sigma_i |x_i|$
- L2 Norm (Euclidean): $||x||_2 = \sqrt{(\Sigma_i x_i^2)}$
- L ∞ Norm (Max): $||x|| \infty = \max_i |x_i|$

Matrix Operations

Matrix Multiplication:

C = AB where
$$C_{ij}$$
 = $\Sigma_k A_{ik}B_{kj}$

Matrix Transpose:

$$(A^T)_{ij} = A_{ji}$$

Matrix Inverse:

$$AA^{-1} = A^{-1}A = I$$

where I is the identity matrix

Eigenvalues and Eigenvectors

For matrix A and vector v:

- λ is the eigenvalue
- v is the eigenvector

Characteristic Equation:

$$det(A - \lambda I) = 0$$

Calculus in ML

Derivatives

Basic Rules:

- Power Rule: $d/dx(x^n) = nx^{n-1}$
- Chain Rule: $d/dx[f(g(x))] = f'(g(x)) \times g'(x)$
- Product Rule: d/dx[f(x)g(x)] = f'(x)g(x) + f(x)g'(x)

Partial Derivatives

For function f(x,y):

```
\partial f/\partial x = partial derivative with respect to x \partial f/\partial y = partial derivative with respect to y
```

Gradient

For function $f(x_1, x_2, ..., x_n)$:

$$\nabla f = [\partial f/\partial x_1, \partial f/\partial x_2, ..., \partial f/\partial x_n]^T$$

Gradient Descent Update Rule

$$\theta_{t+1} = \theta_t - \alpha \nabla f(\theta_t)$$

- θ: parameters
- α: learning rate
- ∇f: gradient of loss function

Hessian Matrix

Second-order partial derivatives:

$$H(f)_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

Probability Theory

Basic Probability

```
P(A) \in [0, 1]

P(\Omega) = 1 (probability of sample space)

P(\emptyset) = 0 (probability of empty set)
```

Conditional Probability

$$P(A|B) = P(A \cap B) / P(B)$$

P(A|B): probability of A given B

Bayes' Theorem

$$P(A|B) = [P(B|A) \times P(A)] / P(B)$$

Extended form:

$$P(A|B) = [P(B|A) \times P(A)] / [\Sigma_i P(B|A_i) \times P(A_i)]$$

Probability Distributions

Bernoulli Distribution:

$$P(X = x) = p^{x}(1-p)^{1-x} \text{ for } x \in \{0,1\}$$

Binomial Distribution:

$$P(X = k) = C(n,k) \times p^{k} \times (1-p)^{n-k}$$

where C(n,k) = n!/(k!(n-k)!)

Normal (Gaussian) Distribution:

$$f(x) = (1/\sqrt{(2\pi\sigma^2)}) \times exp(-(x-\mu)^2/(2\sigma^2))$$

Multivariate Normal:

$$f(x) = (1/((2\pi)^{(k/2)}|\Sigma|^{(1/2)})) \times \exp(-\%(x-\mu)^{T}\Sigma^{-1}(x-\mu))$$

- Σ: covariance matrix
- $|\Sigma|$: determinant of Σ

Expectation and Variance

Expectation (Expected Value):

- Discrete: $E[X] = \Sigma_x x \times P(X = x)$
- Continuous: $E[X] = \int x \times f(x) dx$

Variance:

$$Var(X) = E[(X - E[X])^2] = E[X^2] - (E[X])^2$$

Information Theory

Entropy

For discrete variable X:

$$H(X) = -\Sigma_i P(X_i) \times log_2(P(X_i))$$

- Measures uncertainty/information content
- Units: bits (log₂) or nats (ln)

Cross-Entropy

Between distributions P and Q:

$$H(P,Q) = -\Sigma_i P(X_i) \times log(Q(X_i))$$

Kullback-Leibler (KL) Divergence

$$KL(P|Q) = \Sigma_i P(x_i) \times log(P(x_i)/Q(x_i))$$

- Measures difference between distributions
- $KL(P||Q) \neq KL(Q||P)$ (not symmetric)

Mutual Information

Loss Functions

Regression Loss Functions

Mean Squared Error (MSE):

MSE =
$$(1/n) \times \Sigma_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Mean Absolute Error (MAE):

$$MAE = (1/n) \times \Sigma_{i=1}^{n} |y_{i} - \hat{y}_{i}|$$

Huber Loss (Robust to outliers):

```
\begin{array}{lll} L_{-}\delta(y,\hat{y}) &=& \{ & & \\ & \cancel{2}(y-\hat{y})^2 & & \text{if } |y-\hat{y}| \leq \delta \\ & & \delta|y-\hat{y}| - \cancel{2}\delta^2 & & \text{if } |y-\hat{y}| > \delta \\ \} \end{array}
```

Classification Loss Functions

Binary Cross-Entropy (Log Loss):

$$BCE = -(1/n) \times \Sigma_{i=1}^{n} \left[y_{i} log(\hat{y}_{i}) + (1-y_{i}) log(1-\hat{y}_{i}) \right]$$

Categorical Cross-Entropy (Multi-class):

$$CCE = -(1/n) \times \Sigma_{i=1}^{n} \Sigma_{j=1}^{m} y_{ij}log(\hat{y}_{ij})$$

- m: number of classes
- y_{ij}: 1 if sample i belongs to class j, 0 otherwise

Hinge Loss (SVM):

$$L = \max(0, 1 - y \times \hat{y})$$

Optimization Algorithms

Gradient Descent Variants

Batch Gradient Descent:

$$\theta = \theta - \alpha \times (1/n) \times \Sigma_{i=1}^{n} \nabla \theta L(x_{i}, y_{i}, \theta)$$

Stochastic Gradient Descent (SGD):

$$\theta = \theta - \alpha \times \nabla \theta L(x_i, y_i, \theta)$$

Mini-batch Gradient Descent:

$$\theta = \theta - \alpha \times (1/m) \times \Sigma_{i=1}^{m} \nabla \theta L(x_i, y_i, \theta)$$

Advanced Optimizers

Momentum:

$$\begin{aligned} v_t &= \beta v_{t-1} + \alpha \nabla \theta L \\ \theta_t &= \theta_{t-1} - v_t \end{aligned}$$

RMSprop:

$$S_{t} = \beta S_{t-1} + (1-\beta)(\nabla \theta L)^{2}$$

$$\theta_{t} = \theta_{t-1} - \alpha \times \nabla \theta L / \sqrt{(S_{t} + \epsilon)}$$

Adam (Adaptive Moment Estimation):

$$\begin{array}{lll} m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla \theta L & (1 \text{st moment}) \\ v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla \theta L)^2 & (2 \text{nd moment}) \\ \hat{m}_t = m_t / (1 - \beta_1^{\, t}) & (\text{bias correction}) \\ \hat{v}_t = v_t / (1 - \beta_2^{\, t}) & (\text{bias correction}) \\ \theta_t = \theta_{t-1} - \alpha \times \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon) \end{array}$$

Linear Models Mathematics

Linear Regression

Model:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_n x_n = x^T \beta$$

Normal Equation (Closed-form solution):

$$\beta = (X^T X)^{-1} X^T y$$

Cost Function (MSE):

$$J(\beta) = (1/2n) \times \Sigma_{i=1}^{n} (y_i - x_i^T \beta)^2$$

Gradient:

$$\nabla \beta J = -(1/n) \times X^{T}(y - X\beta)$$

Ridge Regression (L2 Regularization)

Cost Function:

$$J(\beta) = (1/2n) \times \Sigma_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda ||\beta||_2^2$$

Solution:

$$\beta = (X^TX + \lambda I)^{-1}X^Ty$$

Lasso Regression (L1 Regularization)

Cost Function:

$$J(\beta) = (1/2n) \times \Sigma_{i=1}^{n} (y_i - x_i^{\mathsf{T}}\beta)^2 + \lambda ||\beta||_1$$

- No closed-form solution
- Solved using coordinate descent or proximal gradient

Logistic Regression

Sigmoid Function:

$$\sigma(z) = 1/(1 + e^{-z})$$

Model:

$$P(y=1|x) = \sigma(x^T\beta) = 1/(1 + e^{-x^T\beta})$$

Log-Likelihood:

```
LL = \Sigma_{i=1}^{n} [y_i log(\sigma(x_i^{\mathsf{T}}\beta)) + (1-y_i) log(1-\sigma(x_i^{\mathsf{T}}\beta))]
```

Gradient:

$$\nabla \beta LL = X^{T}(y - \sigma(X\beta))$$

Tree-Based Models Mathematics

Decision Trees

Gini Impurity:

Gini = 1 -
$$\Sigma_{j=1}^c$$
 p_j^2

- c: number of classes
- p_i: proportion of samples in class j

Entropy:

Entropy =
$$-\Sigma_{j=1}^{c} p_{j} \log_{2}(p_{j})$$

Information Gain:

IG = Entropy(parent) -
$$\Sigma_i$$
 (n_i/n) × Entropy(child_i)

- n_i: number of samples in child i
- n: total samples in parent

Variance Reduction (for regression):

$$VR = Var(parent) - \Sigma_i (n_i/n) \times Var(child_i)$$

Random Forest

Prediction (Regression):

$$\hat{y} = (1/B) \times \Sigma_{\beta=1}^{B} T_{\beta}(x)$$

- B: number of trees
- T_β: prediction from tree b

Prediction (Classification):

$$\hat{y} = mode\{T_1(x), T_2(x), ..., T^B(x)\}$$

Feature Importance:

Importance_j =
$$(1/B) \times \Sigma_{\beta=1}^{B} \Sigma_{t} \in_{\beta} 1(v(t)=j) \times p(t)\Delta_{it}$$

- v(t): variable used at node t
- p(t): proportion of samples reaching node t
- Δ_{it}: impurity decrease at node t

Gradient Boosting

Additive Model:

$$F(x) = \sum_{m=1}^{M} \gamma_m h_m(x)$$

Update Rule:

$$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x)$$

Gradient Calculation:

$$r_{im} = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F=F_{m-1}}$$

Support Vector Machines Mathematics

Hard Margin SVM

Objective:

```
minimize: %||w||^2
subject to: y_i(w^Tx_i + b) \ge 1 for all i
```

Soft Margin SVM

Objective:

minimize:
$$2||w||^2 + C \times \Sigma_i \xi_i$$

subject to: $y_i(w^Tx_i + b) \ge 1 - \xi_i$
 $\xi_i \ge 0$

- ξ_i: slack variables
- C: regularization parameter

Kernel Trick

Kernel Function:

$$K(x, x') = \phi(x)^T \phi(x')$$

Common Kernels:

- Linear: $K(x, x') = x^Tx'$
- Polynomial: $K(x, x') = (\gamma x^T x' + r)^d$
- RBF (Gaussian): $K(x, x') = \exp(-\gamma ||x x'||^2)$
- Sigmoid: $K(x, x') = \tanh(\gamma x^T x' + r)$

Dual Form Prediction:

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i K(x_i, x) + b$$

Neural Network Mathematics

Forward Propagation

Linear Transformation:

$$z^{(1)} = W^{(1)}a^{(1-1)} + b^{(1)}$$

Activation:

$$a^{(1)} = g^{(1)}(z^{(1)})$$

Activation Functions

ReLU (Rectified Linear Unit):

$$ReLU(z) = max(0, z)$$

Leaky ReLU:

LeakyReLU(z) =
$$max(\alpha z, z)$$
 where $\alpha \approx 0.01$

Sigmoid:

$$\sigma(z) = 1/(1 + e^{-z})$$

Tanh:

$$tanh(z) = (e^{z} - e^{-z})/(e^{z} + e^{-z})$$

Softmax (Multi-class output):

$$softmax(z_i) = e^(z_i) / \Sigma_j e^(z_j)$$

Backpropagation

Chain Rule Application:

$$9\Gamma/9M_{(1)} = 9\Gamma/9S_{(1)} \times 9S_{(1)}/9M_{(1)}$$

Error Propagation:

$$\delta^{(1)} = (W^{(1+1)})^{T}\delta^{(1+1)} \odot g'(z^{(1)})$$

• ①: element-wise multiplication

Weight Update:

$$W^{(1)} = W^{(1)} - \alpha \times \delta^{(1)}(a^{(1-1)})^{T}$$

Batch Normalization

Normalization:

$$\hat{x}_i = (x_i - \mu B)/\sqrt{(\sigma B^2 + \epsilon)}$$

Scale and Shift:

$$y_i = \gamma \hat{x}_i + \beta$$

• γ, β: learnable parameters

Dropout

Training:

$$a^{(1)} = a^{(1)} \odot m^{(1)} / p$$

- m⁽¹⁾: binary mask (Bernoulli(p))
- p: keep probability

Clustering Mathematics

K-Means

Objective Function:

$$J = \Sigma_{i=1}^{n} \sum_{k=1}^{K} r_{ik} | |x_i - \mu_k| |^2$$

• r_{ik}: 1 if x_i belongs to cluster k, 0 otherwise

Update Rules:

$$\begin{array}{l} \mu_k = (\Sigma_i \ r_{ik} x_i)/(\Sigma_i \ r_{ik}) \quad \text{(centroid update)} \\ r_{ik} = 1 \ \text{if} \ k = \text{argmin_j} \ ||x_i - \mu_j||^2 \quad \text{(assignment)} \end{array}$$

DBSCAN

Core Point:

$$|N\epsilon(p)| \ge minPts$$

• $N\epsilon(p) = \{q \in D \mid dist(p,q) \le \epsilon\}$

Density-Reachable:

• p is reachable from q if there's a chain of core points

Gaussian Mixture Models

Probability Model:

$$p(x) = \Sigma_{k=1}^{K} \pi_k \times N(x | \mu_k, \Sigma_k)$$

E-step (Expectation):

```
\gamma_{ik} = (\pi_k \times N(x_i | \mu_k, \Sigma_k))/(\Sigma_j \pi_j \times N(x_i | \mu_j, \Sigma_j))
```

M-step (Maximization):

```
\begin{split} \pi_k &= (1/n) \times \Sigma_i \ \gamma_{ik} \\ \mu_k &= (\Sigma_i \ \gamma_{ik} X_i) / (\Sigma_i \ \gamma_{ik}) \\ \Sigma_k &= (\Sigma_i \ \gamma_{ik} (X_i \ - \ \mu_k) (X_i \ - \ \mu_k)^\top) / (\Sigma_i \ \gamma_{ik}) \end{split}
```

Dimensionality Reduction Mathematics

Principal Component Analysis (PCA)

Objective: Find projection that maximizes variance

Covariance Matrix:

$$C = (1/n) \times X^T X$$

Eigendecomposition:

 $C = V \Lambda V^T$

- V: eigenvectors (principal components)
- Λ: eigenvalues (diagonal matrix)

Projection:

 $Z = XV_k$

• V_k: first k eigenvectors

Reconstruction:

$$\hat{X} = ZV_k^T$$

Explained Variance Ratio:

EVR =
$$\lambda_i$$
 / Σ_j λ_j

Linear Discriminant Analysis (LDA)

Between-class Scatter:

SB =
$$\Sigma_k n_k (\mu_k - \mu) (\mu_k - \mu)^T$$

Within-class Scatter:

$$Sw = \Sigma_k \Sigma_i \in C_k (x_i - \mu_k)(x_i - \mu_k)^T$$

Objective:

Solution: Eigenvectors of Sw⁻¹SB

t-SNE

Joint Probability (High-dimensional):

$$p_{ij} = (p_j|_i + p_i|_j)/(2n)$$

where:

$$p_{j}|_{i} = \exp(-||x_{i} - x_{j}||^{2}/(2\sigma_{i}^{2})) / \Sigma_{k} \neq_{i} \exp(-||x_{i} - x_{k}||^{2}/(2\sigma_{i}^{2}))$$

Joint Probability (Low-dimensional):

$$q_{ij} = (1 + ||y_i - y_j||^2)^{-1} / \Sigma_k \neq_l (1 + ||y_k - y_l||^2)^{-1}$$

Cost Function (KL divergence):

$$C = KL(P||Q) = \Sigma_i \Sigma_j p_{ij} \log(p_{ij}/q_{ij})$$

Evaluation Metrics Mathematics

Classification Metrics

Confusion Matrix Elements:

- TP: True Positives
- TN: True Negatives
- FP: False Positives
- FN: False Negatives

Accuracy:

Accuracy =
$$(TP + TN)/(TP + TN + FP + FN)$$

Precision:

Precision =
$$TP/(TP + FP)$$

Recall (Sensitivity, True Positive Rate):

Recall =
$$TP/(TP + FN)$$

Specificity (True Negative Rate):

Specificity =
$$TN/(TN + FP)$$

F1 Score:

F-beta Score:

$$F\beta = (1 + \beta^2) \times (Precision \times Recall)/((\beta^2 \times Precision) + Recall)$$

Matthews Correlation Coefficient:

$$MCC = (TP \times TN - FP \times FN) / \sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}$$

ROC and AUC

ROC Curve: Plot of TPR vs FPR at various thresholds

AUC (Area Under ROC Curve):

$$AUC = \int_0^1 TPR(FPR) dFPR$$

Approximation (Trapezoidal Rule):

AUC
$$\approx \Sigma_i \% (TPR_i + TPR_{i+1}) (FPR_{i+1} - FPR_i)$$

Regression Metrics

R² Score (Coefficient of Determination):

$$R^2 = 1 - (SS_res/SS_tot)$$

where:

SS_res =
$$\Sigma_i$$
 $(y_i - \hat{y}_i)^2$ (residual sum of squares)
SS_tot = Σ_i $(y_i - \bar{y})^2$ (total sum of squares)

Adjusted R²:

$$R^2$$
_adj = 1 - [(1- R^2)(n-1)/(n-p-1)]

• p: number of predictors

Mean Absolute Percentage Error (MAPE):

MAPE =
$$(100/n) \times \Sigma_i |y_i - \hat{y}_i|/|y_i|$$

Clustering Metrics

Silhouette Score:

$$s(i) = (b(i) - a(i))/max(a(i), b(i))$$

where:

- a(i): average distance to points in same cluster
- b(i): minimum average distance to points in other clusters

Davies-Bouldin Index:

DB =
$$(1/k) \times \Sigma_{i=1}^{k} \max_{j \neq i} [(\sigma_i + \sigma_j)/d(c_i, c_j)]$$

- σ_i: average distance of points in cluster i to centroid
- d(c_i, c_j): distance between centroids

Calinski-Harabasz Index:

CH =
$$[tr(B_k)/(k-1)] / [tr(W_k)/(n-k)]$$

• B_k: between-group dispersion matrix

Additional Important Formulas

Regularization

Elastic Net (L1 + L2):

$$J(\theta) = L(\theta) + \lambda_1 ||\theta||_1 + \lambda_2 ||\theta||_2^2$$

Distance Metrics

Euclidean Distance:

$$d(x,y) = \sqrt{(\Sigma_i (x_i - y_i)^2)}$$

Manhattan Distance:

$$d(x,y) = \Sigma_i |x_i - y_i|$$

Cosine Similarity:

$$cos(x,y) = (x \cdot y)/(||x||_2 \times ||y||_2)$$

Minkowski Distance:

$$d(x,y) = (\Sigma_i | x_i - y_i|^p)^{(1/p)}$$

Bias-Variance Decomposition

Total Error:

$$E[(y - \hat{y})^2] = Bias^2 + Variance + Irreducible Error$$

where:

Bias =
$$E[\hat{y}] - y$$

Variance = $E[(\hat{y} - E[\hat{y}])^2]$

Cross-Validation Error

k-Fold CV Error:

$$CV(k) = (1/k) \times \Sigma_{i=1}^{k} L(h_i, D_i)$$

- h_i: model trained on all folds except i
- D_i: validation data from fold i

Time Series Analysis

Autoregressive (AR) Model

$$y_t = c + \Sigma_{i=1}^p \varphi_i y_{t-i} + \epsilon_t$$

- φ_i: AR coefficients
- p: order of AR model

Moving Average (MA) Model

$$y_t = \mu + \epsilon_t + \Sigma_{i=1}^g \theta_i \epsilon_{t-i}$$

- θ_i: MA coefficients
- q: order of MA model

ARIMA Model

$$(1 - \Sigma_{i=1}^{p} \phi_{i}L^{i})(1-L)^{d}y_{t} = (1 + \Sigma_{i=1}^{g} \theta_{i}L^{i})\epsilon_{t}$$

- L: lag operator
- d: degree of differencing

Exponential Smoothing

Simple: $\alpha y_t + (1-\alpha)\hat{y}_{t-1}$ Double: $\alpha y_t + (1-\alpha)(\hat{y}_{t-1} + \hat{b}_{t-1})$ Triple (Holt-Winters): Includes seasonal component

Autocorrelation Function (ACF)

$$\rho_k = Cov(y_t, y_{t-k}) / Var(y_t)$$

Partial Autocorrelation Function (PACF)

Correlation between y_t and y_{t-k} after removing effects of intermediate lags

Bayesian Methods

Bayes' Rule (Full Form)

$$P(\theta|D) = P(D|\theta)P(\theta) / P(D)$$

- $P(\theta|D)$: Posterior
- P(D|θ): Likelihood
- $P(\theta)$: Prior
- P(D): Evidence

Maximum A Posteriori (MAP)

$$\theta_{MAP} = \operatorname{argmax}_{\theta} P(\theta|D) = \operatorname{argmax}_{\theta} P(D|\theta)P(\theta)$$

Bayesian Linear Regression

Posterior:

$$P(w|D) = N(w|\mu_n, \Sigma_n)$$

where:

$$\Sigma_{n} = (\Sigma_{0}^{-1} + \beta X^{T}X)^{-1}$$

 $\mu_{n} = \Sigma_{n}(\Sigma_{0}^{-1}\mu_{0} + \beta X^{T}y)$

Variational Inference

ELBO (Evidence Lower Bound):

$$L(q) = Eq[log P(X,Z)] - Eq[log q(Z)]$$

Markov Chain Monte Carlo (MCMC)

Metropolis-Hastings Accept Probability:

$$\alpha = \min(1, P(\theta'|D)Q(\theta|\theta') / P(\theta|D)Q(\theta'|\theta))$$

Convolutional Neural Networks

Convolution Operation

$$(f * g)[n] = \Sigma_m f[m] \times g[n-m]$$

2D Convolution (Images)

$$S(i,j) = (I * K)(i,j) = \Sigma_m \Sigma_n I(m,n)K(i-m,j-n)$$

- I: input image
- K: kernel/filter

Pooling

Max Pooling:

```
y = max(x_1, x_2, ..., x_n) in pooling window
```

Average Pooling:

```
y = (1/n)\Sigma_i \times_i in pooling window
```

Output Size Calculation

Output Size =
$$[(W - F + 2P)/S] + 1$$

- W: input size
- F: filter size
- P: padding
- S: stride

Number of Parameters

Conv Layer: $(F \times F \times C_{in} + 1) \times C_{out}$ FC Layer: $(N_{in} + 1) \times N_{out}$

Recurrent Neural Networks

Vanilla RNN

$$\begin{aligned} h_t &= \text{tanh}\big(W_{hh}h_{t-1} + W_{\times h}X_t + b_h\big) \\ y_t &= W_{h\gamma}h_t + b_\gamma \end{aligned}$$

LSTM (Long Short-Term Memory)

Forget Gate:

```
f_t = \sigma(Wf \cdot [h_{t-1}, x_t] + bf)
```

Input Gate:

```
 i_t = \sigma(Wi \cdot [h_{t-1}, x_t] + bi) 
 \tilde{C}_t = tanh(WC \cdot [h_{t-1}, x_t] + bC)
```

Cell State Update:

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

Output Gate:

$$o_t = \sigma(Wo \cdot [h_{t-1}, x_t] + bo)$$

 $h_t = o_t * tanh(C_t)$

GRU (Gated Recurrent Unit)

Update Gate: $z_t = \sigma(Wz \cdot [h_{t-1}, x_t])$ Reset Gate: $r_t = \sigma(Wr \cdot [h_{t-1}, x_t])$ Hidden State: $h_t = (1-z_t)h_{t-1} + z_t\tilde{h}_t$

Transformer Architecture

Scaled Dot-Product Attention

Attention(Q,K,V) = softmax(QK $^{T}/\sqrt{d_k}$)V

- Q: Query matrix
- K: Key matrix
- V: Value matrix
- d_k: dimension of keys

Multi-Head Attention

```
MultiHead(Q,K,V) = Concat(head_1,...,head_h)W^0
```

where:

$$head_{i} = Attention(QW_{i}^{\psi}, KW_{i}^{\kappa}, VW_{i}^{v})$$

Positional Encoding

```
PE(pos,2i) = sin(pos/10000^(2i/d_model))
PE(pos,2i+1) = cos(pos/10000^(2i/d_model))
```

Layer Normalization

$$LN(x) = \gamma \times (x-\mu)/\sqrt{(\sigma^2+\epsilon)} + \beta$$

Recommender Systems

Collaborative Filtering

Matrix Factorization:

 $R \approx PQ^T$

- R: user-item rating matrix
- P: user feature matrix
- Q: item feature matrix

Objective Function:

min
$$\Sigma(i,j) \in K (r_{ij} - p_i^T q_j)^2 + \lambda(||p_i||^2 + ||q_j||^2)$$

Cosine Similarity

$$sim(u,v) = (\Sigma_i r_{ui}r_{vi}) / (\sqrt{\Sigma_i} r_{ui}^2 \times \sqrt{\Sigma_i} r_{vi}^2)$$

Pearson Correlation

$$sim(u,v) = \Sigma_i(r_{ui} - \bar{r}_u)(r_{vi} - \bar{r}_v) / \sqrt{(\Sigma_i(r_{ui} - \bar{r}_u)^2 \times \Sigma_i(r_{vi} - \bar{r}_v)^2)}$$

Reinforcement Learning Mathematics

Bellman Equation

For Value Function:

$$V(s) = \max_{a} [R(s,a) + \gamma \Sigma_{s'} P(s'|s,a)V(s')]$$

For Q-Function:

$$Q(s,a) = R(s,a) + \gamma \Sigma_s' P(s'|s,a) \max_a' Q(s',a')$$

Policy Gradient Theorem

$$\nabla \theta J(\theta) = E[\nabla \theta \log \pi \theta(a|s) \times Q\pi(s,a)]$$

Temporal Difference Learning

TD(0):

$$V(s_t) \leftarrow V(s_t) + \alpha[r_{t+1} + \gamma V(s_{t+1}) - V(s_t)]$$

 $TD(\lambda)$:

$$V(s) \leftarrow V(s) + \alpha \delta_t e_t(s)$$

where eligibility trace:

$$e_t(s) = \gamma \lambda e_{t-1}(s) + 1(s=s_t)$$

Actor-Critic

Critic Update: Update value function V(s) **Actor Update**: $\nabla \theta J = E[\nabla \theta \log \pi \theta(a|s) \times A(s,a)]$ where advantage A(s,a) = Q(s,a) - V(s)

Statistical Hypothesis Testing

Z-Test

$$z = (\bar{x} - \mu) / (\sigma/\sqrt{n})$$

T-Test

One Sample:

$$t = (\bar{x} - \mu) / (s/\sqrt{n})$$

Two Sample (Equal Variance):

$$t = (\bar{x}_1 - \bar{x}_2) / (s_p V(1/n_1 + 1/n_2))$$

where pooled variance:

$$s_p^2 = ((n_1-1)s_1^2 + (n_2-1)s_2^2) / (n_1+n_2-2)$$

Chi-Square Test

$$\chi^2 = \Sigma_i (O_i - E_i)^2 / E_i$$

- O_i: observed frequency
- E_i: expected frequency

ANOVA F-Statistic

```
F = MSB / MSW = (SSB/(k-1)) / (SSW/(n-k))
```

- MSB: mean square between groups
- MSW: mean square within groups

p-value

```
p-value = P(|Test Statistic| ≥ |Observed Value| | H₀)
```

Ensemble Methods Mathematics

Bagging

Bootstrap Sampling: Sample n instances with replacement **Aggregation**: $\hat{y} = (1/B)\Sigma_{\beta} f_{\beta}(x)$

AdaBoost

Sample Weight Update:

$$W_i^{(t+1)} = W_i^{(t)} \times exp(-\alpha_t y_i h_t(x_i))$$

Classifier Weight:

$$\alpha_t = \frac{1}{2} \log((1-\epsilon_t)/\epsilon_t)$$

Final Prediction:

$$H(x) = sign(\Sigma_t \alpha_t h_t(x))$$

Gradient Boosting Mathematics

Pseudo-Residuals:

$$r_{im} = -[\partial L(y_i, f(x_i))/\partial f(x_i)]_{f=f_{m-1}}$$

Line Search:

$$\gamma_m = argmin_\gamma \Sigma_i L(y_i, f_{m-1}(x_i) + \gamma h_m(x_i))$$

XGBoost Objective

$$L = \Sigma_i \ 1(y_i, \hat{y}_i) + \Sigma_k \ \Omega(f_k)$$

where:

$$\Omega(f) = \gamma T + \frac{1}{2}\lambda ||w||^2$$

- T: number of leaves
- w: leaf weights

Graph Neural Networks

Graph Convolution

$$H^{(1+1)} = \sigma(\tilde{D}^{-1}/{}^{2}\tilde{A}\tilde{D}^{-1}/{}^{2}H^{(1)}W^{(1)})$$

- $\tilde{A} = A + I$ (adjacency matrix with self-loops)
- D: degree matrix of A

Message Passing

$$h_{i}^{(k+1)} = \sigma(W_{sel}fh_{i}^{(k)} + \Sigma_{j} \in N(i) W_{nei}g_{h}h_{j}^{(k)})$$

Graph Attention

$$\alpha_{ij} = softmax_{j}(LeakyReLU(a^{T}[Wh_{i}||Wh_{j}]))$$

Advanced Optimization

Newton's Method

$$\theta_{t+1} = \theta_t - H^{-1}\nabla f(\theta_t)$$

• H: Hessian matrix

L-BFGS

Approximates inverse Hessian using limited memory

Conjugate Gradient

$$d_{k+1} = -g_{k+1} + \beta_k d_k$$

where:

$$\beta_k = g_{k+1}^T g_{k+1} / g_k^T g_k$$
 (Fletcher-Reeves)

Natural Gradient

$$\theta_{t+1} = \theta_t - \alpha F^{-1} \nabla L(\theta_t)$$

• F: Fisher Information Matrix

Sampling Methods

Rejection Sampling

Accept x with probability:

$$p(accept) = f(x) / (M \times g(x))$$

Importance Sampling

$$E_p[f(x)] = E_q[f(x)p(x)/q(x)]$$

Gibbs Sampling

Sample each variable conditioned on others:

$$X_i^{(t+1)} \sim P(X_i | X_1^{(t+1)}, ..., X_{i-1}^{(t+1)}, X_{i+1}^{(t)}, ..., X_n^{(t)})$$

Online Learning

Stochastic Gradient Descent

$$\theta_{t+1} = \theta_t - \eta_t \nabla l(x_t, y_t, \theta_t)$$

Online Gradient Descent Regret Bound

Regret
$$\leq |\theta^*|^2/(2\eta) + \eta \times \Sigma_t |g_t|^2/2$$

Exponential Weighted Average

$$W_{t+1,i} = W_{t,i} \times exp(-\eta l_{t,i}) / Z_t$$

Semi-Supervised Learning

Self-Training Loss

$$L = \Sigma_{l} L(x_{l}, y_{l}) + \lambda \Sigma_{u} L(x_{u}, \hat{y}_{u})$$

Graph-Based SSL

Label Propagation:

$$f_{t+1} = \alpha W f_t + (1-\alpha) y$$

Co-Training

Train two classifiers on different views:

$$h_1: X_1 \rightarrow Y$$

$$h_2: X_2 \rightarrow Y$$

Probabilistic Graphical Models

Hidden Markov Models (HMM)

Forward Algorithm:

$$\alpha_t(j) = [\Sigma_i \ \alpha_{t-1}(i)a_{ij}] \times b_j(o_t)$$

- a_{ij}: transition probability
- b_j(o_t): emission probability

Backward Algorithm:

$$\beta_t(i) = \Sigma_j \ a_{ij}b_j(o_{t+1})\beta_{t+1}(j)$$

Viterbi Algorithm:

$$\delta_t(j) = \text{max}_i [\delta_{t-1}(i) \times a_{ij}] \times b_j(o_t)$$

Baum-Welch Update:

$$a_{ij} = \Sigma_t \xi_t(i,j) / \Sigma_t \gamma_t(i)$$

Conditional Random Fields (CRF)

$$P(y|x) = (1/Z(x)) \times exp(\Sigma_t \Sigma_k \lambda_k f_k(y_{t-1}, y_t, x, t))$$

- Z(x): partition function
- f_k: feature functions
- λ_k : weights

Belief Propagation

Message Update:

$$m_{i} \rightarrow_{j} (x_{j}) = \Sigma_{xi} \psi_{i}(x_{i}) \psi_{ij}(x_{i}, x_{j}) \Pi_{k} \in N(i) \setminus j m_{k} \rightarrow_{i} (x_{i})$$

More Probability Distributions

Poisson Distribution

$$P(X = k) = (\lambda^{k}e^{-\lambda}) / k!$$

• Mean = Variance = λ

Exponential Distribution

$$f(x) = \lambda e^{-\lambda^{x}} \text{ for } x \ge 0$$

- Mean = $1/\lambda$
- Variance = $1/\lambda^2$

Gamma Distribution

$$f(x) = (\beta^{\alpha}/\Gamma(\alpha)) \times x^{\alpha-1}e^{-\beta^{\times}}$$

Beta Distribution

$$f(x) = (x^{\alpha-1}(1-x)^{\beta-1}) / B(\alpha, \beta)$$

where $B(\alpha, \beta) = \Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha+\beta)$

Dirichlet Distribution

$$f(x_1,...,x_k) = (1/B(\alpha)) \times \Pi_i \times_i \alpha^{i-1}$$

Student's t-Distribution

$$f(x) = \Gamma((v+1)/2) / (\sqrt{(v\pi)}\Gamma(v/2)) \times (1 + x^2/v)^{-(v+1)/2}$$

Laplace Distribution

$$f(x) = (1/2b) \times exp(-|x-\mu|/b)$$

Anomaly Detection

Gaussian Anomaly Detection

Anomaly Score:

$$f(x) = \exp(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu))$$

Anomaly if $f(x) < \varepsilon$

Isolation Forest

Path Length:

$$h(x) = E[path length to isolate x]$$

Anomaly Score:

$$s(x,n) = 2^{-E(h(x))/c(n)}$$

Local Outlier Factor (LOF)

$$LOF(x) = (\Sigma_{\gamma} \in N(x) lrd(y)) / (|N(x)| \times lrd(x))$$

• Ird: local reachability density

One-Class SVM

min
$$(1/2)||w||^2 + (1/vn)\Sigma_i \xi_i - \rho$$

subject to: $w \cdot \phi(x_i) \ge \rho - \xi_i$

Mahalanobis Distance

$$D(x) = \sqrt{((x-\mu)^T S^{-1}(x-\mu))}$$

Active Learning

Uncertainty Sampling

Least Confident:

$$x^* = \operatorname{argmax}_x [1 - P(\hat{y}|x)]$$

Margin Sampling:

$$x^* = \operatorname{argmin}_{x} [P(\hat{y}_1|x) - P(\hat{y}_2|x)]$$

Entropy-Based:

$$x^* = argmax_x [-\Sigma_i P(y_i|x)log P(y_i|x)]$$

Query by Committee

Vote Entropy:

$$x^* = argmax_x [-\Sigma_i (V(y_i)/C)log(V(y_i)/C)]$$

- V(y_i): votes for class i
- C: committee size

Expected Model Change

Multi-Task Learning

Hard Parameter Sharing Loss

$$L = \sum_{t=1}^{T} \alpha_t L_t(f_t(x; \theta_{\text{sharea}}, \theta_t), y^{(t)})$$

Multi-Task Gaussian Process

$$f \sim GP(0, K \otimes K_t)$$

- K: covariance between inputs
- K_t: covariance between tasks

Task Uncertainty Weighting

$$L = \Sigma_t (1/2\sigma_t^2)L_t + \log \sigma_t$$

Meta-Learning

Model-Agnostic Meta-Learning (MAML)

Inner Loop:

$$\theta'_{i} = \theta - \alpha \nabla \theta L_{i}(f\theta)$$

Outer Loop:

$$\theta = \theta - \beta \nabla \theta \Sigma_{i} L_{i}(f\theta'_{i})$$

Prototypical Networks

Prototype:

$$c_k = (1/|S_k|) \times \Sigma(x_i,y_i) \in S_k f\phi(x_i)$$

Prediction:

$$P(y=k|x) = \exp(-d(f\phi(x),c_k)) / \Sigma_k' \exp(-d(f\phi(x),c_k'))$$

Reptile Algorithm

$$\theta = \theta + \epsilon(\theta^- - \theta)$$

where θ is obtained after k steps of SGD

Federated Learning

FedAvg Algorithm

Local Update:

$$W_k^{t+1} = W_k^t - \eta \nabla F_k(W_k^t)$$

Global Aggregation:

$$w^{t+1} = \Sigma_{k=1}^{K} (n_k/n) w_k^{t+1}$$

Differential Privacy in FL

$$\tilde{W} = W + N(0, \sigma^2 S^2 I)$$

- S: sensitivity
- σ: noise scale

Fairness Metrics

Demographic Parity

$$P(\hat{Y}=1|A=0) = P(\hat{Y}=1|A=1)$$

Equalized Odds

$$P(\hat{Y}=1|A=0,Y=y) = P(\hat{Y}=1|A=1,Y=y) \text{ for } y \in \{0,1\}$$

Equal Opportunity

$$P(\hat{Y}=1|A=0,Y=1) = P(\hat{Y}=1|A=1,Y=1)$$

Disparate Impact

DI =
$$P(\hat{Y}=1|A=0) / P(\hat{Y}=1|A=1)$$

Fair if DI ≥ 0.8

Individual Fairness

$$d(f(x_1), f(x_2)) \le Ld(x_1, x_2)$$

Causal Inference

Average Treatment Effect (ATE)

$$\tau = E[Y(1) - Y(0)]$$

Propensity Score

$$e(x) = P(T=1|X=x)$$

Inverse Probability Weighting

$$\tau_{i} = (1/n) \Sigma_{i} [T_{i} Y_{i} / e(X_{i}) - (1-T_{i}) Y_{i} / (1-e(X_{i}))]$$

Doubly Robust Estimator

$$\tau_{\rm DR} \, = \, (1/n) \Sigma_{\rm i} \, \left[\mu_{\rm 1}(X_{\rm i}) \, - \, \mu_{\rm 0}(X_{\rm i}) \, + \, T_{\rm i}(Y_{\rm i} - \mu_{\rm 1}(X_{\rm i})) / e(X_{\rm i}) \, - \, (1 - T_{\rm i})(Y_{\rm i} - \mu_{\rm 0}(X_{\rm i})) / (1 - e(X_{\rm i})) \right]$$

Instrumental Variables

$$\hat{\beta}IV = Cov(Y,Z) / Cov(X,Z)$$

Additional Important Concepts

Rademacher Complexity

$$\hat{R}_n(F) = E_\sigma[\sup_{f \in F} (1/n)\Sigma_i \sigma_i f(x_i)]$$

• σ_i: Rademacher random variables

VC Dimension

For hypothesis class H:

• VCD(H) = largest set size that can be shattered

PAC Learning Bound

$$P(|R(h) - \hat{R}(h)| > \varepsilon) \le 2exp(-2n\varepsilon^2)$$

Margin Theory (SVM)

Generalization Bound:

$$R(f) \le \hat{R}_{\gamma}(f) + O(\sqrt{d/\gamma^2 n})$$

Spectral Clustering

Graph Laplacian:

$$L = D - W$$

Normalized Laplacian:

$$L_{norm} = I - D^{-1}/^{2}WD^{-1}/^{2}$$

Gaussian Processes

Prior:

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

Posterior:

$$f^*|X,y,X^* \sim N(\mu^*, \Sigma^*)$$

where:

$$\mu^* = K^{*T}(K+\sigma^2I)^{-1}y$$

 $\Sigma^* = K^{**} - K^{*T}(K+\sigma^2I)^{-1}K^*$

Variational Autoencoders (VAE)

ELBO:

$$L = Eq(z|x)[log p(x|z)] - KL(q(z|x)||p(z))$$

Generative Adversarial Networks (GAN)

Objective:

$$min_G max_D V(D,G) = Ex~pdata[log D(x)] + Ez~pz[log(1-D(G(z)))]$$

Wasserstein Distance

$$\texttt{W(P,Q)} = \inf_{\{\gamma \in \Pi(P,Q)\}} \; \texttt{E(x,y)} \sim \gamma[||x-y||]$$