

## 2. DT KNN

### Decision Tree

#### Impurity Measures:

**Misclassification rate:**  $i_{\text{G}}(t) = 1 - \max_c \pi_c$

**Entropy (Shannon):**  $i_H(t) = -\sum_i \pi_{ci} \log_2 \pi_{ci}$

**Gini index:**  $i_G(t) = 1 - \sum_i \pi_{ci}^2$

**Greedy Optimization:** Use  $i_H(t)$  or  $i_G(t)$  (not  $i_E(t)$ , which doesn't decrease impurity)

#### Information Gain:

$$I_{\text{left}} = \frac{N_{\text{left}}}{N}, \quad I_{\text{right}} = \frac{N_{\text{right}}}{N}$$

$$\Delta i = i(t) - I_{\text{left}} - I_{\text{right}} = i(t) - I_{\text{left}}$$

**Stopping Conditions:**  $i(t) = 0 / \text{dmaz} / N_{\text{node}} < \text{tn} / \Delta i(s, t) < \text{ts}$

**LOOCV:** Equivalent to  $N$ -fold cross-validation

### KNN

Prediction:  $\hat{y} = \arg \max_c \sum_i x_i \in N_k(x) \mathbb{I}(y_i = c)$

#### Distance Metrics:

**L1 (Manhattan):**  $d(x_1, x_2) = \sum_i |x_{1d} - x_{2d}|$

**L2 (Euclidean):**  $d(x_1, x_2) = \sqrt{\sum_i (x_{1d} - x_{2d})^2}$

**L $\infty$ :**  $d(x_1, x_2) = \max_d |x_{1d} - x_{2d}|$

**Cosine Similarity:**  $\text{Sim}(x_1, x_2) = \frac{x_1^T x_2}{\|x_1\| \|x_2\|}$

**Mahalanobis Distance:**  $\sqrt{(x_1 - x_2)^T \Sigma^{-1} (x_1 - x_2)}$  (positive semi-definite, symmetric)

**Weighted KNN** (inverse distance weighting, closer points more important):

$$\hat{y} = \arg \max_c \frac{1}{k} \sum_i x_i \in N_k(x) \frac{1}{d(x_i, x)} \mathbb{I}(y_i = c)$$

#### Hyperparameter Selection:

$k$  small  $\rightarrow$  overfitting

$k$  large  $\rightarrow$  underfitting

Use odd number to avoid ties

**Scale Issue:** Normalization  $x_f = \frac{x_i - \mu_i}{\sigma_i}$  (or use weighted distance)

### Confusion Matrix

Ground \ Predict	1	0
1	TP	FN
0	FP	TN

#### Metrics:

**Precision:**  $\frac{TP}{TP+FP}$

**Sensitivity/Recall:**  $\frac{TP}{TP+FN}$

**Accuracy:**  $\frac{TP+TN}{TP+FN+FP+TN}$

**F1 Score:**  $\frac{2 \cdot \text{prec} \cdot \text{rec}}{\text{prec} + \text{rec}}$

### 3. Prob Method

#### Probabilistic Inference

##### Maximum Likelihood Estimation (MLE):

$\theta_{MLE} = \arg \max_{\theta} p(D|\theta)$

$p(D|\theta) = \prod_i^n p(x_i|\theta)$

$E_{MLE} = -\ln p(D|\theta) = -\sum_i^n \ln p(x_i|\theta)$

$\theta_{MLE} = \frac{|T|}{|T|+H|+1|}$

**Maximum A Posteriori (MAP):**

$\theta_{MAP} = \arg \max_{\theta} p(\theta|D)$

$p(\theta|D) \propto p(D|\theta)p(\theta)$

$E_{MAP} = -(\ln|T| + (a-1)\ln\theta - (|H|+b-1)\ln(1-\theta)$

$\theta_{MAP} = \frac{|T|+a-1}{|T|+H|+a+b-2|}$

**When a = b = 1: MAP = MLE**

**Posterior:**  $P(\theta|D) = \text{Beta}(\theta|a+|T|, b+|H|)$

#### Hoeffding's Inequality

$p(\theta_{MLE} - \theta_{\text{true}} \geq \epsilon) \leq 2e^{-2N\epsilon^2} \leq \delta$

#### Bayesian Models

**Predictive Distribution:**  $p(f|D, a, b) = \int_0^1 p(f|\theta)p(\theta|D, a, b)d\theta$

**Fully Bayesian:**  $\theta^* = \frac{|T|+a}{|T|+H|+a+b|} = \text{Ber}(f|\theta)$

#### Conjugate Priors

**Bernoulli** = Beta ( $f_i = (n-1)$ ):

**Likelihood:**  $p(D|\theta) = \theta^k (1-\theta)^{n-k}$

**Prior:**  $\text{Beta}(\theta|a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{a-1} (1-\theta)^{b-1}$

**When to use Bernoulli:** Modeling binary outcome probabilities (success/failure, yes/no, click/no-click);

**Properties:** Support  $\theta \in [0, 1]$ , Parameters  $a, b > 0$  (shape).

Mean  $E[\theta] = \frac{a}{a+b}$ , mode  $\frac{a-1}{a+b-2}$  (for  $a, b > 1$ ), variance  $\frac{ab}{(a+b)^2(a+b+1)}$ .

**When to use Beta:** Modeling any probability/proportion (not necessarily from Bernoulli data). Examples: click-through rates, conversion rates, exam pass rates, market share percentages

#### Poisson = Gamma:

**Likelihood:**  $p(D|\lambda) = \prod_i^n \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}$  (a Poisson distribution becomes Gaussian when the mean is large)

**Prior:**  $p(\lambda) = \frac{\Gamma(\alpha)}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda}$

**Posterior:**  $p(\lambda|D) = \text{Gamma}(\lambda|\alpha + \sum x_i, \beta + N)$

**When to use:** Modeling count data or event rates (arrivals per hour, defects per unit, events per time interval)

**Properties:** Support  $\lambda \in (0, \infty)$ . Parameters  $\alpha > 0$  (shape),  $\beta > 0$  (rate). Mean  $E[\lambda] = \frac{\alpha}{\beta}$ , mode  $\frac{\alpha-1}{\beta}$  (for  $\alpha \geq 1$ ), variance  $\frac{\alpha}{\beta^2}$ .

**When to use Gamma:** Modeling any positive continuous variable (not necessarily from Poisson data). Examples: time between events, product lifetimes, claim sizes, service times.

#### Gaussian = Gaussian:

**Likelihood:**  $p(D|\mu) = \prod_i^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma^2}\right)$

**Prior:**  $p(\mu) = \mathcal{N}(\mu|\mu_0, \tau_0^2)$

**Posterior parameters:**

$\mu_{\text{post}} = (\mu_0\sigma^2 + N\bar{x}_0^2) / (\sigma^2 + N\tau_0^2)$

$$\tau_{\text{post}}^2 = 1 / \left( \frac{1}{\tau_0^2} + \frac{N}{\sigma^2} \right)$$

**When to use:** Modeling continuous measurements with known variance (sensor readings, heights, temperatures, test scores)

**Properties:** Support  $\mu \in (-\infty, \infty)$ . Parameters  $\mu_0$  (prior mean),  $\tau_0^2$  (prior variance),  $\sigma^2$  (known data variance).

Mean  $E[\mu] = \mu_{\text{post}}$ , mode  $\mu_{\text{post}}$  (symmetric), variance  $\tau_{\text{post}}^2$ .

Precision  $\tau_{\text{post}}^{-2} = \tau_0^{-2} + N\sigma^{-2}$  (precisions add).

**Uniform = Pareto:**

**Likelihood:**  $p(D|\theta) = \theta^{-N} \cdot \mathbb{1}_{\max(x_i) \leq \theta}$

**Prior:** Pareto( $\theta|\alpha, \lambda$ )  $= \frac{\alpha^\alpha}{\theta^{\alpha+1}} \cdot \mathbb{1}_{\theta \geq \lambda}$

**When to use Uniform:** Modeling data with a hard, unknown upper bound (where data is equally likely anywhere below the bound). Examples: Serial number analysis (German Tank Problem), estimating maximum physical limits; Properties: Support  $\theta \in [\lambda, \infty)$ . Parameters  $\lambda, \alpha > 0$ .

Mean  $E[\theta] = \frac{\alpha\lambda}{\alpha-1}$  (for  $\alpha > 1$ ), mode  $\lambda$ , variance  $\frac{\alpha\lambda^2}{(\alpha-1)^2(\alpha-2)}$ .

(For  $\alpha \geq 2$ ).

**When to use Pareto:** Modeling heavy-tailed quantities or the distribution of a minimum/maximum threshold.

Examples: Wealth distribution, city populations, or (as here) the belief about the maximum possible value of a Uniform variable.

### 4. Linear Regression

**Model:**  $y_i = f(x_i) + \epsilon_i \sim \mathcal{N}(0, \sigma^2)$

**Least Squares Error:**  $E_{LS} = \frac{1}{2} \sum_i^n (w^T x_i - y_i)^2$

**Optimal Weight:**  $w^* = \arg \min_w E_{LS} = (X^T X)^{-1} X^T y = X^{\dagger} y$

**Non-linear Data (Feature Transformation):**

$* f(x) = w_0 + \sum_{j=1}^M w_j \phi_j(x) = w^T \Phi(x)$

$* \Phi \in \mathbb{R}^{N \times (M+1)}$

$* w^* = (\Phi^T \Phi)^{-1} \Phi^T y = \Phi^{\dagger} y$

**Model Complexity:**

$* \text{High variance} \rightarrow \text{overfit}$

$* \text{High bias} \rightarrow \text{underfit}$

**Ridge Regression:**  $E_{ridge} = \frac{1}{2} \sum_i^n (w^T \Phi(x_i) - y_i)^2 + \frac{\lambda}{2} \|w\|^2$

**Probabilistic Formulation**

**Likelihood:**  $y_i \sim \mathcal{N}(w^T \Phi(x_i), \sigma^2)$ ,  $p(y|X, w, \sigma) = \prod_i^n p(y_i|w, \Phi(x_i), \sigma^2)$

**Negative Log-Likelihood:**

$* E_{ML} = -\ln p(y|X, w, \sigma) = -\ln p(w^T x + \epsilon_i)$

$* E_{ML} = \frac{\partial}{\partial w} \sum_i^n (w^T \Phi(x_i) - y_i)^2 + \frac{\lambda}{2} \|w\|^2$

**Maximum Likelihood Estimators:**

$* w_{ML} = w_{LS} = \Phi^{\dagger} y$

$* \frac{1}{\theta_{ML}} = \frac{1}{\theta_{LS}} = \sum_i^n (w_{ML}^T \Phi(x_i) - y_i)^2$

**With Gaussian Prior:**

$p(w|\sigma) = \mathcal{N}(w|0, \sigma^{-2} I) = \left(\frac{M}{2\pi\sigma^2}\right)^{\frac{M}{2}} \exp\left(-\frac{1}{2\sigma^2} w^T w\right)$  ( $M$ : length of  $w$ )

**MAP Estimation:**

$* E_{MAP} = -\ln p(y|X, w, \sigma) - \ln p(w|\sigma)$

$* E_{MAP} = \frac{\partial}{\partial w} \sum_i^n (w^T \Phi(x_i) - y_i)^2 + \frac{\lambda}{2} \|w\|^2$

**Equivalent to Ridge Regression where  $\lambda = \frac{\sigma}{\beta}$**

$* w^*_{ridge} = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T y$

**Fully Bayesian (Linear Regression)**

**Posterior:**  $p(w|D) = \mathcal{N}(w|\mu, \Sigma)$

$* \mu = \beta \Sigma \Phi^T y$

$* \Sigma^{-1} = \alpha I + \beta \Phi \Phi^T$

**Predictions:**

$* MLE: p(y_{new}|x_{new}, w_{ML}, \beta_{ML}) = \mathcal{N}(\hat{y}_{new}|w_{ML}^T \Phi(x_{new}), \beta_{ML}^{-1})$

$* MAP: p(y_{new}|x_{new}, w_{MAP}, \beta) = \mathcal{N}(\hat{y}_{new}|w_{MAP}^T \Phi(x_{new}), \beta^{-1})$

**Fully Bayesian:**

$p(y_{new}|x_{new}, D) = \mathcal{N}(y_{new}|T \phi(x_{new}), \beta^{-1} + \phi(x_{new})^T \Sigma \phi(x_{new}))$

**Weighted Linear Regression**

Objective (with weight  $r_i$ ):  $E_{weighted} = \frac{1}{2} \sum_i r_i (w^T \Phi(x_i) - y_i)^2$

**Optimal Weight:**  $w^*_{weighted} = (\Phi^T R \Phi)^{-1} \Phi^T R y$

### 5. Linear Classification

**Zero-one Loss:**  $l_{01}(y, \hat{y}) = \sum_i \mathbb{I}(\hat{y}_i \neq y_i)$  (loss for incorrect predictions is 1)

**Hyperplane:**  $f(x) = w^T x + w_0$

**Direction:**  $w$

**Distance from origin:**  $\frac{|w_0|}{\|w\|}$

**Distance to Plane:** The distance from the point  $x$  to the decision boundary:  $\frac{|w^T x + w_0|}{\|w\|}$

**Perceptron Update Rule (for each misclassified  $x_i$ ):**

$w \leftarrow \begin{cases} w + x_i & \text{if } y_i = 1 \\ w - x_i & \text{if } y_i = 0 \end{cases} \quad w_0 \leftarrow \begin{cases} w_0 + 1 & \text{if } y_i = 1 \\ w_0 - 1 & \text{if } y_i = 0 \end{cases}$

**Probabilistic Generative Model:**

**Prior:**  $p(\cdot|y) \sim \text{Categorical}(\theta)$ ,  $p(y=c) = \theta_c = \frac{N_c}{N}, \sum_c \theta_c = 1$

**Class-conditional:**  $p(x|y=c) = \mathcal{N}(x|\mu_c, \Sigma_c)$  (assume  $\Sigma_c$  all equal)

**Probabilistic Generative Models & Discriminant Analysis**

**Remember**  $\sum_{c=1}^C \sum_{n=1}^N = 1$

**Binary Classification:**

$* p(y=1|x) = \sigma(a) = \frac{1}{1+e^{-a}}$  where  $a = \ln \frac{p(x|y=1)p(y=1)}{p(x|y=0)p(y=0)}$

$* a = w^T x + w_0$

**LDA (Linear Discriminant Analysis) (with shared covariance  $\Sigma$ ):**

$* w = \Sigma^{-1}(\mu_1 - \mu_0)$

$* w_0 = -\frac{1}{2} w^T \Sigma^{-1} \mu_1 + \frac{1}{2} w^T \Sigma^{-1} \mu_0 + \ln \frac{p(y=1)}{p(y=0)}$

$* \text{Thus } y|x \sim \text{Bernoulli}(\sigma(w^T x + w_0))$

**Naive Bayes (assumes feature independence):**

$* p(x|y=c) = \prod_{i=1}^d p(x_i|y=c)$

**Gaussian Naive Bayes:**  $p(x_j|y=c) = \mathcal{N}(x_j|\mu_{jc}, \sigma_{jc}^2)$

**Equivalent to LDA/QDA with diagonal covariance matrix**

$* a = w^T x + w_0 \text{ where } w_{ij} = \frac{\mu_{1j} - \mu_{0j}}{\sigma_{0j}^2} - \frac{\mu_{1j}}{\sigma_{1j}^2} \quad (\text{if } \sigma_{1j} = \sigma_{0j})$

**Multinomial Naive Bayes:** for discrete features (e.g., word counts)

$* p(x_j|y=c) = \text{Categorical}(\theta_{jc})$

$* \log p(y=c|x) \propto \sum_i x_i \log \theta_{jc} + \log p(y=c)$

**Bernoulli Naive Bayes:** for binary features

$* p(x_j|y=c) = \text{Bernoulli}(\theta_{jc})$

**Multi-class Classification:**

$* p(y=c|x) = \frac{\exp(w^T x + w_0)}{\sum_j \exp(w^T x + w_j)}$

$* w_c = \Sigma^{-1} \mu_c$

$* w_0 = -\frac{1}{2} \mu_c^T \Sigma^{-1} \mu_c + \ln p(y=c)$

**QDA (Quadratic Discriminant Analysis) (different covariances  $\Sigma_{ij}$ ):**

$* p(y=c|x) = \frac{\exp(w^T x + w_0)}{\sum_j \exp(w^T x + w_j)}$

$* w_c = \Sigma^{-1} \mu_c$

$* w_0 = -\frac{1}{2} \mu_c^T \Sigma^{-1} \mu_c + \ln p(y=c)$

**One hot:**

$* \Pi_{c=1}^C (p_c)^{y_c} = \text{ptrue class}$

$* p(D|y=c) = \prod_{i=1}^C p(x_i|y=c)^{y_i}$

$* \pi_{c=1}^C = \text{all parameters for all } C \text{ classes}$

**Linear Discriminant Model: Logistic Regression**

**Binary Logistic Regression:**

$* p(y=1|x) = \sigma(w^T x)$

$* p(y=0|x) = 1 - \sigma(w^T x)$

$* p(w|x, \theta_{c=1}) = \prod_{i=1}^n \prod_{c=1}^C \text{ptrue class}$

$* \pi_{c=1}^C = \text{all parameters for all } C \text{ classes}$

## 9. Support Vector Machines (SVM)

Margin:  $\frac{w^T x_i + b}{\|w\|}$

Constraints:

- $w^T x_i + b \geq 1$  for  $y_i = +1$
- $w^T x_i + b \leq -1$  for  $y_i = -1$

Thus:  $y_i(w^T x_i + b) - 1 \geq 0$  for  $\forall x_i$

Optimization Problem:

Minimize:  $\frac{1}{2} w^T w$

Subject to:  $f(w, b) = y_i(w^T x_i + b) - 1 \geq 0$

Lagrangian Dual Function

Dual function:  $g(\alpha) = \min_{w \in \mathbb{R}^n} d(f_0(\theta) + \sum_{i=1}^M \alpha_i f_i(\theta))$

Lagrangian:  $L(\theta, \alpha) = f_0(\theta) + \sum_{i=1}^M \alpha_i f_i(\theta)$

Conditions:  $\alpha_i \geq 0$  and  $f_i(\theta) \leq 0$

SVM Optimization Steps

1. Calculate Lagrangian:

$$L(w, b, \alpha) = \frac{1}{2} w^T w - \sum_i^N \alpha_i [y_i(w^T x_i + b) - 1]$$

2. Minimize L:

$$\frac{\partial L}{\partial w} = w - \sum_i^N \alpha_i y_i x_i = 0$$

$$\frac{\partial L}{\partial b} = \sum_i^N \alpha_i y_i = 0$$

$$\Rightarrow w = \sum_i^N \alpha_i y_i x_i$$

3. Dual Problem:

$$g(\alpha) = \sum_i^N \alpha_i - \frac{1}{2} \sum_i^N \sum_j^N y_i y_j \alpha_i \alpha_j x_i^T x_j$$

Note:  $x_i^T x_j$  can be replaced by Kernel  $\Phi(x_i, x_j)$

w.r.t.  $\alpha_i \geq 0$ ,  $\sum_i^N \alpha_i = 0$

$$w = \sum_i^N \alpha_i y_i x_i$$

$$b = \frac{1}{N} y_i - w^T x_i = y_i - w^T x_i$$

$\therefore h(x) = \text{sign}(\sum_i^N \alpha_i y_i x_i^T x + b)$

Soft SVM (relaxed margin):

Constraint:  $y_i(w^T x_i + b) \geq 1 - \xi_i$  ( $\xi_i \geq 0$ )

Minimize:  $f_0(w, b, \xi) = \frac{1}{2} w^T w + C \sum_i^N \xi_i$

w.r.t.:

$$y_i(w^T x_i + b) - 1 + \xi_i \geq 0$$

$\xi_i \geq 0$

( $C \rightarrow \infty$ : hard margin)

Soft Margin SVM Derivation

1. Lagrangian Formulation:

$$L(w, b, \xi, \mu) = \frac{1}{2} w^T w + C \sum_i^N \xi_i - \sum_i^N \alpha_i [y_i(w^T x_i + b) - 1 + \xi_i] - \sum_i^N \mu_i i$$

2. Minimize L (Gradients):

$$\frac{\partial L}{\partial w} = w - \sum_i^N \alpha_i y_i x_i = 0$$

$$\frac{\partial L}{\partial b} = \sum_i^N \alpha_i = 0$$

$$\frac{\partial L}{\partial \xi_i} = C - \alpha_i - \xi_i = 0 \Rightarrow \alpha_i = C - \mu_i$$

Since  $\mu_i \geq 0$  and  $\alpha_i \geq 0$ : Box Constraint  $\alpha_i \in [0, C]$

3. Maximize Dual Function:

$$g(\alpha) = \sum_i^N \alpha_i - \frac{1}{2} \sum_i^N \sum_j^N y_i y_j \alpha_i \alpha_j x_i^T x_j$$

Subject to:

$$\sum_i^N \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C$$

Interpretation of  $\alpha_i$ :

If  $0 < \alpha_i < C$ :  $\xi_i = 0$  and  $y_i(w^T x_i + b) = 1$  (point lies exactly on the margin)

If  $\alpha_i = C$ :  $\xi_i > 0$  (point violates the margin)

If  $0 < \xi_i < 1$ : point is inside the margin but correctly classified

If  $\xi_i \geq 1$ :  $y_i(w^T x_i + b) \leq 0$ , point is misclassified

Larger  $C \rightarrow$  less tolerance for points inside the margin

Hinge Loss:

$$\frac{1}{2} w^T w + C \sum_i^N \max\{0, 1 - y_i(w^T x_i + b)\}$$

Kernel Methods

Definition:  $k(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

Prediction:  $h(x) = \text{sign}(\sum_{j \in S} \alpha_j y_j k(x_i, x_j) + b)$

Kernel Matrix Properties, Mercer: Must be symmetric positive semi-definite

$c^T K c \geq 0$

Sum =  $\sum_i \sum_j c_i c_j k(x_i, x_j) \geq 0$

Valid Kernel Construction Rules:

1. Sum:  $k(x_1, x_2) = k_1 + k_2$

2. Scaling:  $k(x_1, x_2) = ck_1$  with  $c > 0$

3. Product:  $k(x_1, x_2) = k_1 \cdot k_2$

4. Transformation:  $k(x_1, x_2) = k_3(\phi(x_1), \phi(x_2))$

5. Matrix Scaling:  $k(x_1, x_2) = x_1^T A x_2$  where  $A$  is symmetric positive semi-definite

Common Examples:

• Polynomial:  $k(a, b) = (a^T b)^n$  or  $(a^T b + 1)^P$

• Gaussian (RBF):  $k(a, b) = \exp(-\frac{\|a-b\|^2}{2\sigma^2})$

Mercer Theorem: Sum =  $\sum_i \sum_j c_i c_j k(x_i, x_j) \geq 0$  / The Gram matrix must be PSD ( $c^T K c \geq 0$ )  $\rightarrow$  Convexity Section

Multiclass Classification Strategies

• 1 vs n classification: Look at maximum distance

• 1 vs 1 classification: Look at majority vote

## 10. Dimension Reduction PCA SVD

Dimension Reduction (PCA)

Transformation:  $\tilde{x} = \bar{x} - F \cdot \Sigma^{-1}_x = x^T \Sigma_x^{-1} x$

(Minimizing Error = Maximizing Variance)

1. Centering Data

$$\bar{x}_i = x_i - \bar{x} \text{ where } \bar{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} = \frac{1}{N} \cdot X^T \cdot 1_N$$

2. Variance and Covariance

$$\text{Variance: } \text{Var}(X_j) = \frac{1}{N} X_j^T X_j - \bar{x}_j^2$$

$$\text{Covariance: } \text{Cov}(X_j, X_j) = \frac{1}{N} X_j^T X_j - \bar{x}_j \bar{x}_j$$

$$\text{Covariance Matrix: } \Sigma_{\bar{X}} = \frac{1}{N} \bar{X}^T \bar{X} \text{ (symmetric)}$$

3. Eigen-decomposition

$\Sigma_{\bar{X}} = \Gamma \Lambda \Gamma^T$  (where  $\Lambda$  is diagonal)

4. Transformation

$$\bar{x} = X \cdot \Gamma$$

$$Y_{\text{reduced}} = \bar{X} \cdot \Gamma_{\text{truncated}}$$

Reconstruction:  $X_{\text{reconstructed}} = Y_{\text{reduced}} \cdot \Gamma_{\text{truncated}}$  (back to original dims)

Criteria: Retain 90% of variance:  $\sum_{i=1}^k \lambda_i \geq 0.9 \sum_{i=1}^d \lambda_i$

Complexity:  $O(nd^2 + d^3)$

5. Iterative Eigenvector Calculation

Power Iteration:  $v \leftarrow \frac{v}{\|v\|}$  (converges to eigenvector with largest eigenvalue)

Singular Value Decomposition (SVD)

Goal: Find best low-rank approximation of matrix  $A$

Frobenius Norm Objective:  $\|A - B\|_F^2 = \sum_i^N \sum_j^D (a_{ij} - b_{ij})^2$

Complexity:  $O(n \cdot d^2)$  or  $O(n^2 \cdot d)$

Decomposition:  $A = U \Sigma V^T$  where:

•  $U \in \mathbb{R}^{n \times n}$  (user-to-concept similarity)

•  $\Sigma \in \mathbb{R}^{n \times r}$

•  $V \in \mathbb{R}^{r \times D}$  (item-to-concept similarity)

Rank-2 Decomposition:  $A = (\sigma_1 \cdot u_1 \cdot v_1^T) + (\sigma_2 \cdot u_2 \cdot v_2^T)$

EYM

$$A = U \Sigma V^T = \sum_{i=1}^{\min(m,n)} \sigma_i u_i v_i^T$$

Using SVD of Dimensionality Reduction

Projection:  $P = U \Sigma$  or  $P = A \cdot V$

Reconstruction:  $A_{\text{reconstructed}} = U \Sigma V^T$  or

$$A_{\text{reconstructed}} = P \cdot V_k^T$$

Retain 90% energy:  $\sum_{i=1}^k \sigma_i^2 \geq 0.9 \sum_{i=1}^r \sigma_i^2$

Relationship to Eigenvectors:

•  $V$  contains eigenvectors of  $X^T X$

•  $U$  contains eigenvectors of  $XX^T$

SVD vs PCA

• Eigenvectors = Singular Vectors; (N)Eigenvalues = (Singular Values)<sup>1/2</sup>

• Transform the data such that dimensions of new space are uncorrelated + discard (new) dimensions with smallest variance = find optimal low-rank approximation (norm\_F)

Matrix Factorization (MF)

1. Fundamentals & Metrics

2. Alternating Optimization

1. Initialize:  $P_0, Q_0, t = 0$

2. Update  $P$ :  $P_{t+1} = \arg\min_P p(P, Q_t)$

• Closed form:  $p_T = \left( \frac{1}{|S_{*,i}|} \sum_{j \in S_{*,i}} q_{ji} \right)^{-1} \cdot \frac{1}{|S_{*,i}|} \sum_{j \in S_{*,i}} q_{ji}^T r_{ui}$

3. Update  $Q$ :  $Q_{t+1} = \arg\min_Q f(P_{t+1}, Q)$

4. Repeat until convergence

3. Stochastic Gradient Descent (SGD)

•  $e_{ui} \leftarrow r_{ui} - q_{ui} - p_{ui}^T$

•  $q_{ui} \leftarrow q_{ui} + 2r_{ui}e_{ui}$  (learning rate)

•  $p_{ui} \leftarrow p_{ui} + 2r_{ui}e_{ui}$

5. Extensions: Bias & Regularization

Regularized Objective:

$$\sum_i (r_{ui} - q_{ui} - p_{ui}^T)^2 + \lambda_1 \sum_i \|q_{ui}\|^2 + \lambda_2 \sum_i \|p_{ui}\|^2$$

Full Loss with Bias:

$$L = \sum_i (r_{ui} - (q_{ui} + b_u + b_i) + 1)^2 + \lambda_1 \sum_i \|q_{ui}\|^2 + \lambda_2 \sum_i \|p_{ui}\|^2$$

SGD Updates (with Bias & Regularization):

$$1. e_{ui} = r_{ui} - q_{ui} - p_{ui}^T$$

$$2. q_{ui} = q_{ui} + 2r_{ui}e_{ui} - \lambda_1 q_{ui}$$

$$3. p_{ui} = p_{ui} + 2r_{ui}e_{ui} - \lambda_2 p_{ui}$$

$$4. b_u = b_u + 2r_{ui}e_{ui}$$

$$5. b_i = b_i + 2r_{ui}e_{ui}$$

$$6. b = \frac{1}{|S|} \sum_i r_{ui}$$
 (Global Bias)

## 11. Dimension Reduction Neighbor Graph Method

Neighbor Graph Method

Preserve local structure

Scatter Plot (High Dim) vs Adjacency Matrix (Graph)

t-SNE

High-dimensional similarity:

$$(1 + \|y_i - y_j\|^2)^{-1}$$

$$q_{ij} = \frac{1}{\sum_k \sum_{l \neq k} (1 + \|y_i - y_l\|^2)^{-1}}$$

• Target  $y$

$$* q_{ii} = 0$$

Next: minimize KL Divergence

$$\sum_i \sum_{j \neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}} = KL(P||Q)$$

•  $KL(P||Q) \geq 0$  iff  $P = Q$

Divergence Behavior:

$KL(P||Q)$ : Mean-seeking (Covers the whole distribution)

$KL(P||Q)$ : Mode-seeking (Looks onto specific modes)

Autoencoder

Notes:

• Bottleneck ( $L \ll D$ )

• Extract key features and reconstruct; equivalent to only taking  $\text{rank}(X) = L$

• Formula:  $XW_1W_2 = \bar{X}$

$$\cdot W_1W_2 = W^* = \Gamma$$

$\Gamma$  is the largest  $L$  eigenvectors of  $X^T X$ .

## 12. Clustering

K-means: Objective (Distortion Measure)

• Formula:

$$J(X, Z, \mu) = \sum_i^K \sum_{j=1}^K z_{ik} \|x_i - \mu_k\|^2$$

• Indicator Variable:

•  $z_{ik} = \{0, 1, 0, 0, 0\}$  implies sample  $i$  belongs to class  $z$ .

Lloyd's Algorithm (Alternating Optimization)

1. Initialize: All centroids  $\mu_i$ .

2. Assignment: Assign cluster indicators based on the nearest neighbor.

• (Note: Whichever centroid a point is closest to, it belongs to that cluster.)

3. Update:

$$\cdot \mu_k = \frac{1}{N_k} \sum_{i=1}^N z_{ik} x_i$$

• Where  $N_k = \sum_i^N z_{ik}$

4. Loop: Repeat until convergence.

K-means ++

1. Randomly select one data point as  $\mu_1$ .

2. Calculate the distance of the remaining points to it:

$$\|x_i - \mu_1\|^2$$

3. Sample the next center point, with probability proportional to the distance size.

4. Recalculate  $D_i^2 = \min\{\|x_i - \mu_1\|^2, \|x_i - \mu_2\|^2, \dots\}$ .

5. Repeat steps 3 and 4 until  $K$  centers are chosen.

Gaussian Mixture Model (GMM)

Model Definition:

$$p(x|\theta) = \sum_z p(z|\theta)p(x|z)$$

• latent variables

• Optimization Goal:  $\theta^* = \arg\max_{\theta} p(x|\theta)$

Distributions:

1. Prior:  $p(z|\theta) = \text{Cat}(\pi) \quad // \{ \pi_1, \pi_2, \dots, \pi_K \}$

• Constraints:  $\sum_i^K \pi_i = 1$

2. Likelihood:  $p(x|z, \theta) = N(x|\mu_z, \Sigma_z)$

Parameters:

Thus  $\theta = \{\pi, \mu, \Sigma\}$

•  $\pi$ :  $k$  parameters (effectively  $k-1$ )

•  $\mu$ :  $R^d \cdot k \cdot d$  parameters

•  $\Sigma$ :  $R^d \times d \cdot k \cdot d^2$  parameters (or  $k \cdot \frac{d(d+1)}{2}$  due to symmetry)

Using GMM as a Generative Model

1. Sample class according to  $\pi = \{\pi_1, \pi_2, \dots, \pi_K\}$

2. Generate  $x$  according to  $x \sim N(\mu_k, \Sigma_k)$  (Probability Density)

Marginal Probability:

$$p(x|\pi, \mu, \Sigma) = \sum_i^K \pi_i \cdot N(x|\mu_k, \Sigma_k)$$

