Introduction to Data Science

-K-Nearest Neighbors & Naive Bayes Classification -

Mauricio Molina

Keio University, Faculty of Economics

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What Is K-Nearest Neighbors (KNN)?

Predicting qualitative responses is a process that is known as **classification**. Predicting a qualitative response for an observation can be referred to as classifying classification that observation, since it involves assigning the observation to a category, or class.

The **K-Nearest Neighbors** (KNN) method, for example, is quite simple: classify a record in accordance with how similar records are classified.

K-Nearest Neighbors

For each record to be classified or predicted:

- 1. Find K records that have similar features (i.e., similar predictor values).
- 2. For classification, find out what the majority class is among those similar records and assign that class to the new record.
- 3. For prediction (also called KNN regression), find the average among those similar records, and predict that average for the new record.

KNN is one of the simpler prediction/classification techniques: there is no model to be fit. The prediction results depend on how the features are scaled, how similarity is measured, and how big K is set. Also, all predictors must be in numeric form. We will illustrate how to use the KNN method with a classification example.

K-Nearest Neighbors (KNN) Classifier

From a variable-sized dataset, $\mathcal{D} = \{(x_n, y_n) : n = 1, ..., N\}$:

- ullet The KNN classifier assigns a new input ullet to the class most common among its K nearest neighbors in the training set \mathcal{D} .
- Let $\mathcal{N}_K(\mathbf{x}, \mathcal{D})$ denote the set of the K closest examples to \mathbf{x} in \mathcal{D} . Then the class-conditional distribution is

$$p(y = c \mid \mathbf{x}, \mathcal{D}) = \frac{1}{K} \sum_{\mathbf{x}_n \in \mathcal{N}_K(\mathbf{x}, \mathcal{D})} \mathbf{I}(y_n = c).$$

- The two main hyperparameters are:
 - The neighborhood size K.
 - ② The distance metric $d(\mathbf{x}, \mathbf{x}')$.
- Mahalanobis distance:

$$d_M(\mathbf{x}, \boldsymbol{\mu}) = \sqrt{(\mathbf{x} - \boldsymbol{\mu})^{\mathsf{T}} M (\mathbf{x} - \boldsymbol{\mu})},$$

where M is any positive-definite matrix. If M = I, this reduces to the Euclidean distance.

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K-Nearest Neighbors in 2D (K = 5)

- For a new test point x, compute distances to all training points.
- Identify the K = 5 nearest neighbors in feature space.
- Count the labels of those 5 neighbors: here they are {1, 1, 1, 0, 0}.
- Assign **x** to the majority label \rightarrow class "1."
- Hence, we predict $p(y = 1 | \mathbf{x}, \mathcal{D}) = 3/5 = 0.6$

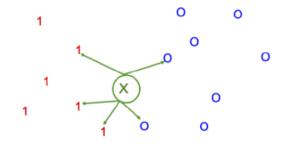


Illustration of a K-nearest neighbors classifier in 2D for K=5. The nearest neighbors of test point \mathbf{x} have labels $\{1,\ 1,\ 1,\ 0,\ 0\}$.



Voronoi Tessellation for 1-NN

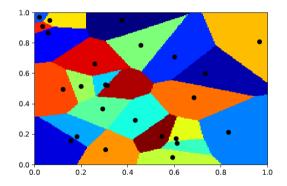


Illustration of the Voronoi tessellation induced by 1-NN

- When K = 1, each training point "owns" the region of the plane where it is the nearest neighbor.
- The resulting partition of feature space is called the Voronoi tessellation.
- A new point is classified according to the single nearest training point.
- Voronoi cells are convex polygons in 2D (generalized to polyhedra in higher dimensions).

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Example on Lending Club data

- Dataset: "loan200" consists of 200 LendingClub personal loans
 - LendingClub is a peer-to-peer lending platform where investors fund individual loans
 - Each loan has a known binary outcome: "paid off" vs. "default" (variable outcome200)

• Predictors:

- dti = Debt-to-Income ratio (excluding mortgage), scaled by 100
- payment_inc_ratio = Loan payment ÷ Income, scaled by 100
- Goal: Given a new loan with

$$dti = 22.5$$
, payment_inc_ratio = 9.0,

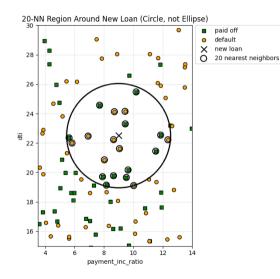
use KNN (with K=20) to predict whether it will "paid off" or "default."

• Procedure:

- Compute distances from the new loan (22.5, 9.0) to all 200 known loans in the 2D feature space
- 2 Identify the 20 nearest neighbors in that feature space
- Assign the new loan to the majority class among those 20 neighbors



KNN Output & Probability Interpretation



- The large black circle shows the boundary of the nearest 20 points. In this case, 9 defaulted loans lie within the circle, as compared with 11 paid-off loans. Hence the predicted outcome of the loan is paid off. Note that if we consider only three nearest neighbors, the prediction would be that the loan defaults.
- Although KNN classification typically returns a binary label ("default" vs. "paid off"), most implementations can also output a probability (propensity) for each class.
- The probability of "default" is simply: number of neighbors labeled "default" divided by K.
- In this example, suppose among the 20 nearest neighbors, 9 have label "default." Then

$$\hat{P}(\text{default} \mid \text{new loan}) = \frac{9}{20} = 0.45.$$



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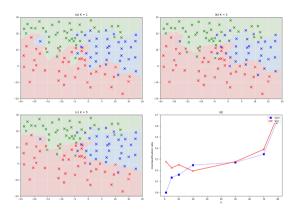


Figure: Decision boundaries induced by a KNN classifier. (a)K=1. (b) K=2. (c) K=5. (d) Train and test error vs K.

As K increases, the decision boundaries become smoother (since we are averaging over larger neighborhoods), so the training error increases, as we start to underfit.

The Curse of Dimensionality

- Main issue: KNN classifiers break down in high dimensions due to the curse of dimensionality.
- Why?
 - In D dimensions, volume grows exponentially fast.
 - To capture a fixed fraction p of the data around a test point x, a hypercube must be very large.

• Example:

- 1 Inputs \mathbf{x} are uniformly distributed in $[0,1]^D$.
- ② Grow a hypercube centered at x until it contains fraction p of points.
- The expected edge length is

$$e_D(p) = p^{1/D}.$$

- Implications for D=10:
 - If p = 0.10, then $e_{10}(0.10) = 0.10^{1/10} \approx 0.80$.
 - If p = 0.01, then $e_{10}(0.01) = 0.01^{1/10} \approx 0.63$.
 - Since each coordinate runs from 0 to 1, a cube of side 0.80 or 0.63 is huge.
- **Key Takeaway:** "Nearest" neighbors lie far away along most dimensions → poor local estimates.

Why Far-Away Neighbors Hurt

- Large hypercubes to capture small $p \Rightarrow$ averaging over a wide region.
- Neighbors may differ drastically in many coordinates.
- Locality vanishes, so KNN no longer "local."

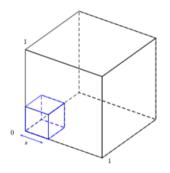
Two Principal Remedies

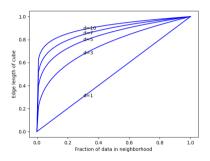
- Use a Parametric Model
 - Impose global structure (e.g., linear or logistic regression, decision trees).
 - Reduces reliance on exponentially large neighborhoods.
- Dimension-Selective Metrics
 - Feature Selection: restrict KNN to a smaller subset of coordinates.
 - Metric Learning / Mahalanobis: weight/transform dimensions so that "closeness" reflects relevance.
 - Effective dimensionality is lowered, neighbors stay truly local.

Summary:

- In low D, KNN is genuinely local.
- As D increases, required edge length $e_D(p) = p^{1/D}$ becomes large.
- Remedy by adding structure (parametric) or reducing/weighting dimensions (metric learning or feature selection).

Curse of Dimensionality





(b) Edge length $e_D(p) = p^{1/D}$ vs. dimension D

- (a) Embedding a small cube of side s inside the unit cube
- (a) A small cube of side s inside a larger unit cube. (b) Plot of $e_D(p)$ vs. D, showing how far the cube must extend in each dimension to capture fraction p.

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Choosing K in KNN

• Importance of *K*:

- K=1 is the 1-nearest neighbor classifier: predict based on the single closest training point.
- In practice, K=1 often overfits; better performance usually achieved with K>1.

• Effects of K:

Small K (e.g., 1) \rightarrow High variance, prone to overfitting and noise. Large K \rightarrow Smoother decision boundary, reduced variance, but risk of *oversmoothing*.

• Choosing the "best" K:

- No universal rule—depends on data structure and noise level (signal-to-noise ratio).
- ullet Use cross-validation or a held-out validation set to compare accuracy for different K.
- Typical range: $K \approx 1$ to 20.
- Often pick an odd K to avoid ties when classes are binary.

Understanding Confusion Matrix

Evaluating Classification Performance

What is a Confusion Matrix?

A table that visualizes classification model performance by comparing predicted vs actual labels. Essential for binary and multi-class classification.

Binary Classification Matrix:

		Actual	
		Positive	Negative
Predicted	Positive	TP	FP
	Negative	FN	TN

Key Components:

- TP (True Positive): Correct positive predictions
- FP (False Positive): Negative cases misclassified as positive (Type I error)
- TN (True Negative): Correct negative predictions
- FN (False Negative): Positive cases misclassified as negative (Type II error)

Performance Metrics:

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

• Precision: $\frac{TP}{TP+FP}$

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

• **F1-score:** $2 \times \frac{Precision \times Recall}{Precision + Recall}$

• Specificity: $\frac{TN}{TN+FP}$

(Overall correctness)

(How accurate positive predictions are)

(Ability to detect positives)

(Harmonic mean of precision/recall)

(Ability to detect negatives)

Bias-Variance Trade-off in KNN

Definitions:

- Variance: Error due to variation in training data. Different training sets yield different models.
- Bias: Error due to model's inability to capture the true underlying structure. Persistence of error even with infinite data.

Trade-off in KNN

- K is too Small:
 - Model is very flexible → low bias.
 - ullet High sensitivity to noise o high variance.
- K is too Large:
 - Model is smoother → low variance.
 - ullet Decision boundary might miss local structure o high bias.
- The "optimal" K balances bias and variance to minimize total error.

Naive Bayes: Overview

- The naive Bayes algorithm uses conditional probabilities $P(X_j \mid Y = k)$ to estimate the posterior probability $P(Y = k \mid X_1, \dots, X_p)$.
- In other words, we want

$$P(Y = k \mid X_1, \dots, X_p)$$

but we start from

$$P(X_1,\ldots,X_p\mid Y=k)$$
 and $P(Y=k)$.

• Key terms:

- Conditional probability: $P(X = x \mid Y = k)$ is the probability that predictor X takes value x given class Y = k.
- Posterior probability: $P(Y = k \mid X_1, ..., X_p)$ is the probability of outcome Y = k after observing predictors. It contrasts with the prior P(Y = k), which ignores predictor values.



- Exact Bayesian classification (conceptual):
 - **1** For a new record with predictors (X_1, \ldots, X_p) , find all training records that match exactly on every predictor.
 - Among those exact matches, determine which class label is most prevalent.
 - Assign that class to the new record.
- This exact approach is like computing

$$P(Y = k \mid X_1, ..., X_p) = \frac{P(Y = k) P(X_1, ..., X_p \mid Y = k)}{\sum_{i=1}^{K} P(Y = i) P(X_1, ..., X_p \mid Y = i)},$$

but only using records with (X_1, \ldots, X_p) exactly equal.

Problem: As the number of categorical predictors increases, the likelihood of finding any training record that matches a new record on *all* predictors goes to zero.

Why Exact Bayesian Classification Fails in Practice

• Example:

- Predict voting by gender, ethnicity, income bracket, region, voting history, number of children, marital status, etc.
- Even a large sample may not contain a single record matching a new record who is, say, male, Hispanic, high-income, Midwest, voted last election, did not vote prior election, three daughters, one son, divorced.
- That is already eight predictors—typical classification problems have many more.
- Adding one more predictor with 5 equally common categories reduces the probability of an exact match by a factor of 5.
- Consequently, most new records have *zero* exact matches \rightarrow cannot estimate $P(X_1, \dots, X_p \mid Y = k)$ by direct counting.



• Naive Bayes remedy: Use the entire dataset but assume conditional independence:

$$P(X_1,\ldots,X_p\mid Y=k) \approx \prod_{j=1}^p P(X_j\mid Y=k).$$

This "naive" assumption lets us compute posterior probabilities even when exact matches do not
exist.



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Using this "naive" assumption, the posterior probability can be computed as:

$$P(Y = k | X_1, ..., X_p) = \frac{P(Y = k) \prod_{j=1}^p P(X_j | Y = k)}{\sum_{i=1}^K P(Y = i) \prod_{j=1}^p P(X_j | Y = i)}$$

We still need to specify the form of the probability distributions for $X_j | Y = k$. This depends on what type of feature X_d is.

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Continuous Variables: Gaussian Naïve Bayes

- **Assumption:** Each continuous feature $X_j \mid Y = k$ follows $\mathcal{N}(\mu_{j,k}, \sigma_{i,k}^2)$.
- Likelihood per feature:

$$f(x_j \mid Y = k) = \frac{1}{\sqrt{2\pi} \sigma_{j,k}} \exp\left(-\frac{(x_j - \mu_{j,k})^2}{2\sigma_{j,k}^2}\right)$$

• Compute parameters $\mu_{j,k}$ and $\sigma_{j,k}$ from training data:

$$\mu_{j,k} = \frac{1}{N_k} \sum_{i:y_i=k} x_{ij}, \quad \sigma_{j,k}^2 = \frac{1}{N_k} \sum_{i:y_i=k} (x_{ij} - \mu_{j,k})^2$$

- Prior $P(Y = k) = \frac{N_k}{N}$.
- Posterior score (log form to avoid underflow):

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Binary Features: Bernoulli Naïve Bayes

- Use case: Binary features (e.g., presence/absence of words in documents, true/false attributes)
- **Assumption:** Each feature $X_i \mid Y = k$ follows Bernoulli distribution:

$$P(X_j = x_j \mid Y = k) = egin{cases} heta_{j,k} & ext{if } x_j = 1 \ 1 - heta_{j,k} & ext{if } x_j = 0 \end{cases}$$

Likelihood for feature vector:

$$P(\mathbf{X} \mid Y = k) = \prod_{j=1}^{p} \theta_{j,k}^{x_j} (1 - \theta_{j,k})^{1-x_j}$$

• Parameter estimation ($\theta_{i,k}$ = probability of feature j being present in class k):

$$\theta_{j,k} = \frac{N_{j,k}}{N_k}$$

where $N_{j,k}=$ number of class k samples with $X_j=1$, $N_k=$ total class k samples

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Bernoulli NB: Handling and Smoothing

- Explicitly models absence of features $(X_j = 0)$
- Posterior probability:

$$P(Y = k \mid \mathbf{X}) \propto P(Y = k) \prod_{j=1}^{p} \theta_{j,k}^{x_j} (1 - \theta_{j,k})^{1-x_j}$$

• Laplace smoothing (essential to prevent zero probabilities):

$$\theta_{j,k} = \frac{N_{j,k} + \alpha}{N_k + 2\alpha}$$

where $\alpha > 0$ (typically $\alpha = 1$)

• **Applications:** Document classification (bag-of-words with binary features), medical diagnosis, binary feature sets

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Count Data: Multinomial Naïve Bayes

- Use case: Discrete frequency counts (e.g., word counts in documents)
- Assumption: Feature vector $\mathbf{X} = (f_1, \dots, f_p)$ follows multinomial distribution
- Likelihood (ignoring constant combinatorial factor):

$$P(\mathbf{X} \mid Y = k) \propto \prod_{j=1}^p \phi_{j,k}^{f_j}$$

where $\phi_{j,k}$ = probability of term j occurring in class k

ullet Normalization constraint: $\sum_{j=1}^p \phi_{j,k} = 1$



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Multinomial NB: Parameter Estimation

• Parameter estimation with Laplace smoothing:

$$\phi_{j,k} = \frac{\sum_{i:y_i=k} f_{ij} + \alpha}{\sum_{i:y_i=k} \left(\sum_{m=1}^{p} f_{im}\right) + \alpha p}$$

- $f_{ij} = \text{count of feature } j \text{ in instance } i$
- $\alpha > 0$ (smoothing parameter, typically $\alpha = 1$)
- p = number of features
- Posterior probability:

$$P(Y = k \mid \mathbf{X}) \propto P(Y = k) \prod_{i=1}^{p} \phi_{j,k}^{f_j}$$

- Key difference from Bernoulli:
 - Multinomial: Uses frequency counts (multiple occurrences matter)
 - Bernoulli: Uses binary presence/absence (multiple occurrences don't matter)

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Multinomial NB: Applications & Notes

- Applications: Text classification, spam detection, categorical data analysis
- Important implementation details:
 - Typically uses log probabilities to avoid underflow
 - Ignores non-occurring features (∏ only over present features)
 - Handles varying document lengths through normalization
- Variant: Complement Naïve Bayes improves performance on imbalanced text datasets

Dataset: "Default.csv" contains 10 000 observations of credit card users.

- ullet Binary outcome default: "Yes" vs. "No" (encoded as default_enc = 1/0)
- Categorical predictor student: "Yes" vs. "No" (encoded as student_enc = 1/0)
- Continuous predictors balance and income

Part 1: Bernoulli Naive Bayes (Student → Default)

- Predictor: $student_enc \in \{0, 1\}$
- Response: $default_enc \in \{0, 1\}$
- Train/test split: 70% train, 30% test, random_state=1, shuffle=True
- Threshold: $P(\text{default} = 1 \mid \text{student_enc}) > 0.2$
- Procedure:
 - Fit BernoulliNB on {student_enc, default_enc}_{train}.
 - ② Compute $P(\text{default} = 1 \mid \text{student_enc} = 0 \text{ or } 1)$.
 - Olassify test point as "default" if its posterior > 0.2, otherwise "no default."
 - Ompute confusion matrix and metrics (accuracy, precision, recall, etc).
- Result (example):

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Part 2: Gaussian Naive Bayes (Balance + Income → Default)

- Predictors: balance and income (continuous)
- ullet Response: default_enc $\in \{0,1\}$
- Train/test split: same 70/30 split as above
- Threshold: $P(\text{default} = 1 \mid \text{balance}, \text{income}) > 0.5$
- Procedure:
 - Fit GaussianNB on {balance, income, default_enc}_{train}.
 - ② Compute posterior $P(\text{default} = 1 \mid \text{balance}, \text{income})$ for each test point.
 - 3 Classify as "default" if posterior > 0.5, else "no default."
 - Compute confusion matrix and metrics (accuracy, precision, recall, etc).
- Result (example):

$$\mbox{Confusion Matrix} = \begin{pmatrix} \textit{TN} & \textit{FP} \\ \textit{FN} & \textit{TP} \end{pmatrix}, \quad \{\mbox{accuracy, precision, recall}, \mbox{F}_1\}$$



Naïve Bayes: Algorithm Comparison

Туре	Feature Space	Likelihood	Parameters
Gaussian Bernoulli	Continuous Binary	Normal Bernoulli	$\mu_{j,k}, \sigma_{j,k} \ heta_{j,k}$
Multinomial	Counts	Multinomial	$\phi_{j,k}$

Shared characteristics:

- Conditional independence assumption
- Requires smoothing for discrete features
- Fast training $(\mathcal{O}(np) \text{ time})$
- Optimal when independence assumption holds
- Weakness: Feature correlation reduces performance



Fundamental Differences

Aspect Naïve Bayes Classifier (NBC)		K-Nearest Neighbors (KNN)	
Туре	Probabilistic generative model Makes distributional assumptions	Instance-based model Makes no distributional assumptions	
Learning	Eager learner: Builds model during training	Lazy learner: Defers computation to prediction time	
Decision	Bayesian decision theory: Chooses class with highest posterior probability	Majority vote: Chooses class most frequent among neighbor	
Assumptions	Conditional feature independence given class (naïve assumption)	Local consistency: Similar inputs have similar outputs	

Advantages & Disadvantages

Naïve Bayes

- + Extremely fast prediction
- + Handles high dimensions well
- + Works with small datasets
- + Naturally handles missing data
- + Probabilistic outputs
- Strong independence assumption
- Poor with correlated features
- Limited representation capacity
- Sensitive to irrelevant features

K-Nearest Neighbors

- + No training time
- + Simple to implement
- + No parametric assumptions
- + Naturally handles multi-modal classes
- Slow prediction time
- Memory intensive
- Sensitive to irrelevant features
- Needs careful distance metric choice
- Curse of dimensionality



When to Use Which?

Choose Naïve Bayes when:

- Real-time prediction is needed
- Training data is large but resources limited
- Features are approximately independent
- Dataset has high dimensionality
- You need probability estimates
- Text classification problems

Choose KNN when:

- Decision boundary is irregular
- You have low-dimensional data
- Dataset size is moderate
- Features are equally important
- You need simple implementation
- Data is noise-free and normalized

Hybrid approach: Use NBC for initial fast screening, KNN for uncertain cases

Practical Performance Comparison

Characteristic	NBC Speed	KNN Speed	NBC Accuracy	KNN Accuracy
Small datasets $(n < 1,000)$	Fast	Fast	Variable	Often high
Large datasets $(n > 100,000)$	Very fast	Slow	Good	Very good
High dimensions $(p > 1,000)$	Excellent	Poor	Good	Poor
Irrelevant features	Sensitive	Sensitive	Degrades	Degrades
Correlated features	Problematic	OK	Degrades	Robust
Non-linear boundaries	Struggles	Excellent	Low	High

Table: Performance characteristics: NBC vs KNN

Note: NBC often outperforms KNN in text classification, while KNN excels in computer vision (with dimensionality reduction) Source: Empirical observations from:

- Zhang, H. (2004). The optimality of Naive Bayes. AA1, 1(2), 3.
- Ocver, T. M., & Hart, P. E. (1967). Nearest neighbor pattern classification. IEEE Transactions on Information Theory, 13(1), 21-27.
- Hand, D. J., & Yu, K. (2001). Idiot's Bayes—not so stupid after all? International Statistical Review, 69(3), 385-398.

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Assignment 12

Answer the following questions in Jupyter Notebook format. Show your code and briefly interpret each result. Upload the completed .ipynb to K-LMS by next Tuesday at midnight.

Q1: KNN on student-mat.csv

- Use G3 as response and {age, Medu, Fedu, traveltime, studytime, failures, famrel, freetime, goout, Dalc, Walc, absences as predictors.
- Split 70/30 (random_state=6), then for $k \in \{1, 3, 5, 7, 9, 11, 13, 15, 17, 19\}$: train a KNeighborsRegressor, record the accuracy on train and test sets.
- Plot k vs. train/test accuracy: identify the k with best test performance.

Q2: Naive Bayes on Default.csv

- Encode default_enc = (default == "Yes") and student_enc = (student == "Yes").
- (a) BernoulliNB: use {student_enc} → default_enc, split 70/30 (random_state=1), threshold 0.6. Report confusion matrix and {accuracy, precision, recall, F1}.
- (b) GaussianNB: use {balance, income} → default_enc, same split, threshold 0.6. Report confusion matrix and metrics
- Compare which feature set yields better classification, and comment on threshold choice.

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