



Лекция № 8

Метод Байеса

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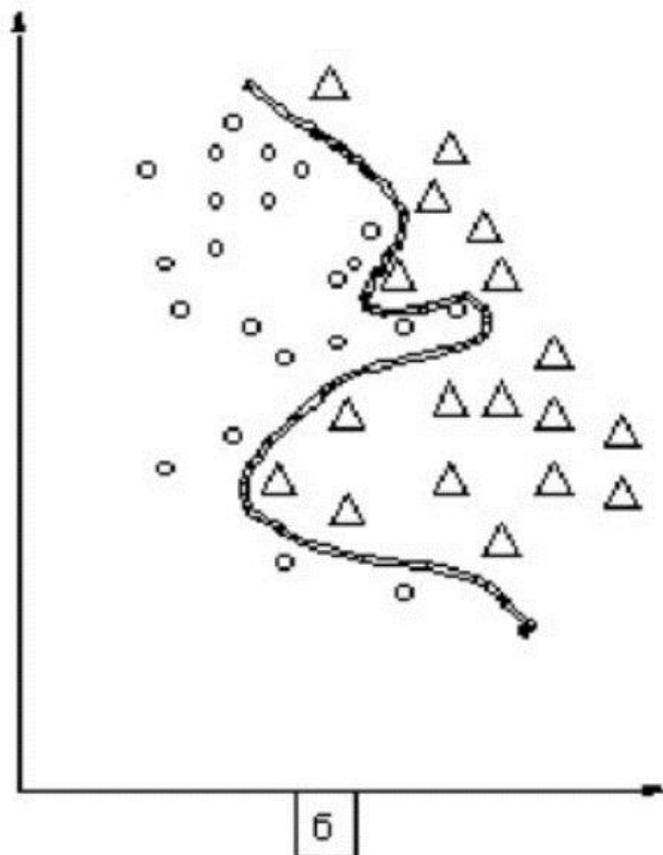
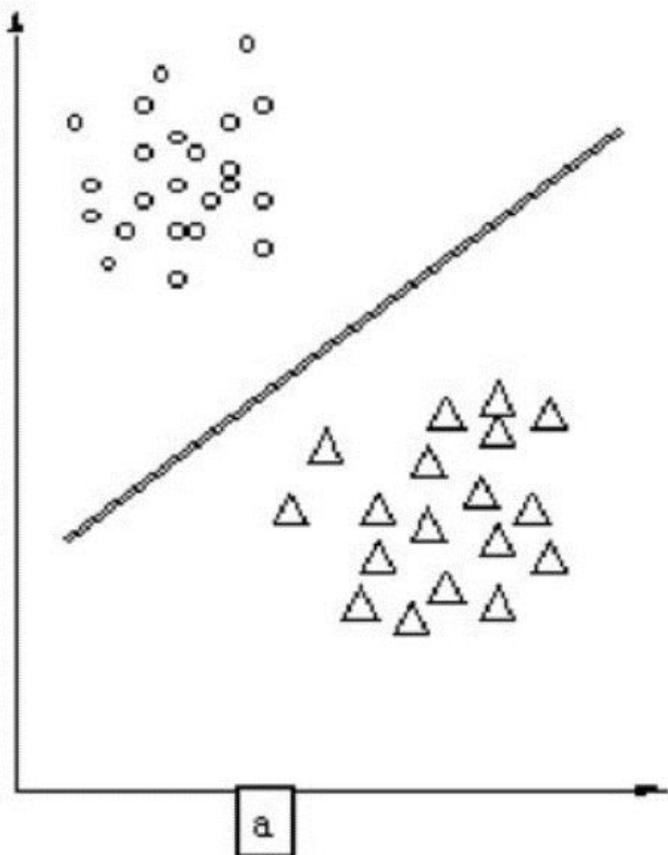
Для студентов, обучающихся по направлению 06.03.01 «Биология»
профили Биохимия, Генетика
при изучении дисциплины «Цифровые технологии в биологии»

П л а н л е к ц и и

- **Что такое метод Байеса**
- **Общая постановка задачи**
- **Функции распределения в методе Байеса**
- **Метод Байеса в программе Statistica**

Задача классификации

Обучение с учителем



Метод Байеса

*Вероятностный центральный
параметрический*

метод классификации

**Основан на последовательном
применении при построении
решающего правила классической
формулы Байеса для условной
вероятности**

Метод Байеса

Апостериорная вероятность события A_k при условии, что наступило событие B

$$P(A_k | B) = \frac{P(B | A_k) \cdot P(A_k)}{\sum_{l=1}^r P(B | A_l) \cdot P(A_l)}$$

$\{A_k\}$ – полная группа попарно несовместных событий с априорными вероятностями

$$P(A_k), k = 1 \dots r$$

B – некоторое событие с вероятностью

$$P(B) > 0$$

Метод Байеса

Для одной переменной $m = 1$ и двух классов $k = a, b$

$$P(A_k | B) = \frac{P(B | A_k) \cdot P(A_k)}{P(B | A_a) \cdot P(A_a) + P(B | A_b) \cdot P(A_b)}$$

Определим прогнозируемое событие как C

Метод Байеса

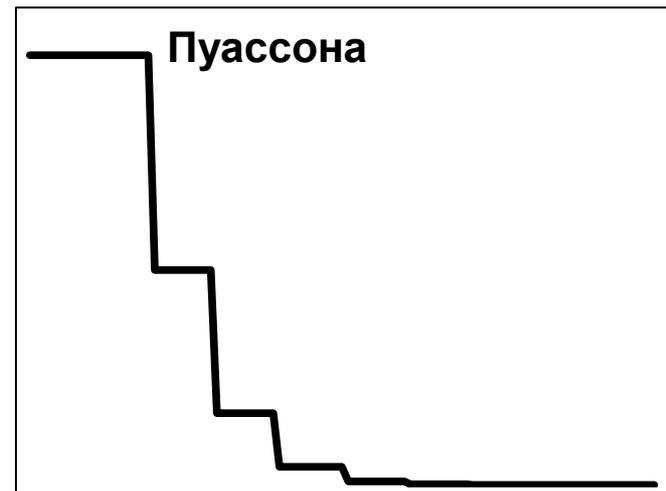
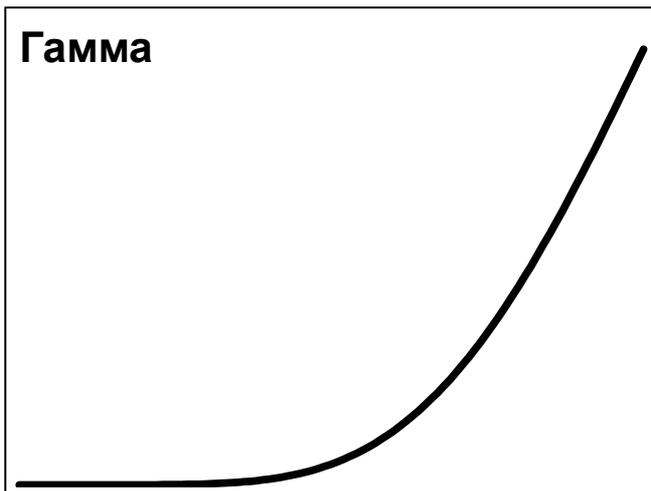
Для m переменных и двух классов $k = a, b$

$$P(C \in k) = \frac{P_0(C \in k) \cdot \prod_{i=1}^m P(B_{ki} | C \in k)}{P_0(C \in a) \cdot \prod_{i=1}^m P(B_{ki} | C \in a) + P_0(C \in b) \cdot \prod_{i=1}^m P(B_{ki} | C \in b)}$$

До начала классификации $P_0(C \in a) = P_0(C \in b) = 0.5$

Метод Байеса

Непрерывные распределения



Метод Байеса

Пример непрерывных исходных данных

| Code | Y3 | Y2 | X1 | X2 | X3 | X4 | X5 | X6 | X7 | X8 | X9 | X10 | X11 | X12 | X13 |
|-------|----------|----|------|------|------|------|------|------|------|------|------|------|------|------|------|
| LT-47 | high | h | -8.5 | -6.5 | -7.9 | -7.1 | -8.2 | -8.7 | -8.3 | -6.2 | -6.7 | -7.5 | -8.5 | -6.4 | -6.3 |
| LT-51 | high | h | -8.4 | -6.7 | -7.4 | -6.6 | -8.1 | -8.6 | -8.3 | -6.1 | -6.5 | -7.4 | -8.4 | -6.8 | -6.1 |
| LT-52 | high | h | -8.6 | -7.1 | -8.2 | -7.0 | -9.4 | -9.2 | -8.6 | -6.4 | -6.8 | -8.2 | -8.6 | -7.5 | -6.4 |
| L-91 | high | h | -8.6 | -6.9 | -6.9 | -8.3 | -9.2 | -8.7 | -8.9 | -6.1 | -6.4 | -7.5 | -8.2 | -7.0 | -6.3 |
| LT-13 | high | h | -8.6 | -7.2 | -8.2 | -7.2 | -9.0 | -8.9 | -8.7 | -6.3 | -6.5 | -7.5 | -8.2 | -6.4 | -5.8 |
| LT-23 | high | h | -8.5 | -6.8 | -7.0 | -7.7 | -8.8 | -8.2 | -8.4 | -6.1 | -6.4 | -7.6 | -8.1 | -7.0 | -6.0 |
| LT-48 | high | h | -8.5 | -6.4 | -7.4 | -6.8 | -8.4 | -8.6 | -8.2 | -6.2 | -6.6 | -7.6 | -8.0 | -6.6 | -6.1 |
| LT-46 | high | h | -8.2 | -6.2 | -7.8 | -7.8 | -7.9 | -8.3 | -7.9 | -6.0 | -6.4 | -7.4 | -8.2 | -6.2 | -6.0 |
| H-16 | high | h | -8.3 | -6.5 | -7.1 | -6.6 | -8.0 | -8.1 | -8.1 | -5.7 | -6.1 | -7.3 | -8.0 | -6.6 | -6.4 |
| H-88 | high | h | -8.6 | -7.0 | -7.3 | -8.0 | -9.3 | -8.4 | -8.0 | -6.1 | -6.4 | -7.2 | -7.9 | -6.8 | -6.3 |
| LT-22 | high | h | -8.5 | -6.9 | -7.4 | -8.3 | -9.0 | -8.3 | -8.4 | -6.0 | -6.3 | -7.5 | -8.2 | -6.8 | -6.5 |
| LT-49 | high | h | -9.0 | -6.6 | -7.0 | -6.8 | -8.4 | -8.5 | -8.4 | -6.0 | -6.3 | -7.6 | -8.0 | -6.3 | -6.3 |
| L-87 | moderate | nh | -8.5 | -7.0 | -7.5 | -7.8 | -8.6 | -8.5 | -8.9 | -6.2 | -6.4 | -7.3 | -8.2 | -6.9 | -6.3 |
| LT-55 | moderate | nh | -8.6 | -7.0 | -7.5 | -7.3 | -8.5 | -8.3 | -9.1 | -6.1 | -6.4 | -7.8 | -8.1 | -6.7 | -6.0 |
| LT-9 | moderate | nh | -8.6 | -6.8 | -7.4 | -8.0 | -8.4 | -8.2 | -8.4 | -6.1 | -6.4 | -6.9 | -7.7 | -6.3 | -6.0 |
| L-20 | moderate | nh | -8.4 | -6.6 | -7.1 | -7.3 | -8.2 | -8.3 | -8.1 | -6.0 | -6.3 | -7.4 | -8.1 | -6.6 | -6.1 |
| L-31 | moderate | nh | -8.4 | -6.9 | -7.4 | -7.8 | -8.0 | -8.4 | -8.1 | -6.2 | -6.6 | -7.4 | -8.0 | -6.4 | -6.6 |
| L-86 | moderate | nh | -8.3 | -6.8 | -6.8 | -8.5 | -8.9 | -8.2 | -8.6 | -6.1 | -6.2 | -7.2 | -8.0 | -6.9 | -6.2 |
| LT-21 | moderate | nh | -8.6 | -6.8 | -7.1 | -8.2 | -8.8 | -8.2 | -8.1 | -6.0 | -6.2 | -7.3 | -8.0 | -6.9 | -6.1 |
| LTG-2 | moderate | nh | -7.8 | -6.8 | -6.9 | -7.3 | -7.9 | -8.0 | -7.4 | -6.2 | -6.5 | -8.1 | -8.4 | -6.9 | -6.8 |
| L-19 | moderate | nh | -8.3 | -6.6 | -7.1 | -6.7 | -8.3 | -8.1 | -7.9 | -6.2 | -6.4 | -7.6 | -7.9 | -6.6 | -6.1 |
| LT-24 | moderate | nh | -8.8 | -7.1 | -6.8 | -7.9 | -8.8 | -8.5 | -8.2 | -5.9 | -6.3 | -7.4 | -7.9 | -6.5 | -6.4 |
| LT-33 | moderate | nh | -8.0 | -6.1 | -7.2 | -7.0 | -7.9 | -7.9 | -7.7 | -5.8 | -5.9 | -7.1 | -8.0 | -6.1 | -5.5 |
| L-17 | moderate | nh | -8.0 | -6.6 | -7.4 | -8.3 | -8.1 | -7.9 | -7.8 | -6.1 | -6.3 | -7.4 | -8.0 | -6.5 | -6.0 |
| LT-34 | moderate | nh | -8.2 | -6.3 | -7.6 | -6.5 | -8.3 | -8.1 | -7.9 | -6.0 | -6.3 | -7.1 | -8.1 | -6.3 | -6.1 |
| LT-36 | moderate | nh | -8.2 | -6.3 | -7.1 | -6.2 | -7.8 | -8.1 | -7.7 | -5.8 | -6.0 | -7.0 | -8.1 | -6.7 | -5.9 |
| LT-50 | moderate | nh | -8.7 | -6.6 | -7.4 | -6.8 | -8.3 | -8.5 | -7.9 | -6.2 | -6.4 | -7.5 | -7.9 | -5.9 | -6.4 |
| LT-5 | moderate | nh | -8.5 | -6.5 | -7.1 | -8.0 | -8.1 | -7.9 | -8.0 | -5.8 | -6.2 | -7.0 | -7.5 | -6.1 | -5.6 |
| H-18 | moderate | nh | -8.6 | -6.7 | -6.8 | -6.6 | -8.2 | -8.0 | -8.2 | -6.1 | -6.3 | -7.4 | -7.9 | -6.3 | -6.4 |
| H-69 | low | nh | -8.2 | -6.5 | -7.1 | -6.5 | -8.0 | -8.1 | -8.1 | -5.9 | -6.2 | -7.4 | -7.8 | -6.3 | -6.4 |
| LT-30 | low | nh | -7.6 | -6.1 | -6.5 | -7.2 | -7.8 | -7.2 | -7.5 | -5.6 | -6.0 | -7.0 | -7.5 | -6.0 | -6.1 |
| LT-31 | low | nh | -7.8 | -6.1 | -6.1 | -5.9 | -7.8 | -7.2 | -7.3 | -5.6 | -5.9 | -7.1 | -7.6 | -6.1 | -5.7 |
| LT-35 | low | nh | -8.1 | -6.2 | -7.0 | -6.5 | -8.5 | -8.2 | -8.0 | -6.0 | -6.3 | -7.0 | -7.8 | -6.6 | -5.9 |
| LT-39 | low | nh | -8.2 | -6.2 | -6.7 | -6.3 | -8.4 | -8.1 | -8.2 | -5.7 | -6.1 | -7.3 | -7.6 | -6.2 | -5.8 |
| LT-29 | low | nh | -7.3 | -5.9 | -6.3 | -6.8 | -7.7 | -6.8 | -7.2 | -5.6 | -5.8 | -7.1 | -7.2 | -6.0 | -5.8 |
| LT-32 | low | nh | -7.7 | -6.2 | -6.0 | -6.7 | -7.6 | -7.3 | -7.6 | -5.3 | -5.7 | -7.0 | -7.4 | -6.1 | -5.8 |
| LT-38 | low | nh | -9.3 | -6.4 | -7.1 | -6.0 | -8.2 | -8.2 | -8.1 | -5.9 | -6.2 | -7.2 | -7.6 | -6.3 | -5.8 |
| LT-37 | low | nh | -9.3 | -6.3 | -7.0 | -6.2 | -8.3 | -8.1 | -8.1 | -5.9 | -6.2 | -7.1 | -7.7 | -6.5 | -5.7 |
| H-42 | low | nh | -7.4 | -6.0 | -6.2 | -6.4 | -7.5 | -7.3 | -7.0 | -5.4 | -5.6 | -7.0 | -7.3 | -6.3 | -5.8 |
| LT-53 | low | nh | -7.5 | -6.1 | -6.3 | -6.8 | -7.4 | -7.4 | -7.2 | -5.6 | -5.9 | -7.0 | -7.4 | -6.3 | -5.9 |
| H-29 | low | nh | -7.1 | -5.5 | -6.2 | -7.6 | -7.1 | -7.1 | -6.7 | -5.3 | -5.6 | -6.6 | -6.8 | -5.9 | -5.5 |

Метод Байеса

STATISTICA - [Data: Docking TDAz_L17* (15v by 43c)]

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Automated Neural Networks
Machine Learning (Bayesian, Support Vectors, Nearest Neighbor)

- General Classification/Regression Tree Models
- General CHAID Models
- Interactive Trees (C&RT, CHAID)
- Boosted Tree Classifiers and Regression
- Random Forests for Regression and Classification
- Generalized Additive Models
- MARSplines (Multivariate Adaptive Regression Splines)
- Generalized EM & k-Means Cluster Analysis
- Independent Components Analysis
- Text & Document Mining, Web Crawling - Methods
- Association Rules
- Sequence, Association, and Link Analysis
- Rapid Deployment of Predictive Models (PMML)
- Goodness of Fit, Classification, Prediction
- Feature Selection and Variable Screening
- Combining Groups (Classes) for Predictive Data Mining
- Data Mining - Workspaces
- QC Data Mining & Root Cause Analysis - Methods

| | LDA | | | | | | | | | | | | | | |
|-------|----------|----|------|------|------|------|------|------|------|------|------|------|------|------|------|
| | 1 | 2 | 3 | | | | | | | | | | | | |
| | Y3 | Y2 | X1 | | | | | | | | | | | | |
| | | | | 12 | 13 | 14 | 15 | | | | | | | | |
| | | | | X10 | X11 | X12 | X13 | | | | | | | | |
| LT-47 | high | h | -8.5 | -7.5 | -8.5 | -6.4 | -6.3 | | | | | | | | |
| LT-51 | high | h | -8.4 | -7.4 | -8.4 | -6.8 | -6.1 | | | | | | | | |
| LT-52 | high | h | -8.6 | -8.2 | -8.6 | -7.5 | -6.4 | | | | | | | | |
| L-91 | high | h | -8.6 | -7.5 | -8.2 | -7.0 | -6.3 | | | | | | | | |
| LT-13 | high | h | -8.6 | -7.5 | -8.2 | -6.4 | -5.8 | | | | | | | | |
| LT-23 | high | h | -8.5 | -7.6 | -8.1 | -7.0 | -6.0 | | | | | | | | |
| LT-48 | high | h | -8.5 | -7.6 | -8.0 | -6.6 | -6.1 | | | | | | | | |
| LT-46 | high | h | -8.2 | -7.4 | -8.2 | -6.2 | -6.0 | | | | | | | | |
| H-16 | high | h | -8.3 | -7.3 | -8.0 | -6.6 | -6.4 | | | | | | | | |
| H-88 | high | h | -8.6 | -7.2 | -7.9 | -6.8 | -6.3 | | | | | | | | |
| LT-22 | high | h | -8.5 | -7.5 | -8.2 | -6.8 | -6.5 | | | | | | | | |
| LT-49 | high | h | -9.0 | -7.6 | -8.0 | -6.3 | -6.3 | | | | | | | | |
| L-87 | moderate | nh | -8.5 | -7.3 | -8.2 | -6.9 | -6.3 | | | | | | | | |
| LT-55 | moderate | nh | -8.6 | -7.8 | -8.1 | -6.7 | -6.0 | | | | | | | | |
| LT-9 | moderate | nh | -8.6 | -6.9 | -7.7 | -6.3 | -6.0 | | | | | | | | |
| L-20 | moderate | nh | -8.4 | -7.4 | -8.1 | -6.6 | -6.1 | | | | | | | | |
| L-31 | moderate | nh | -8.4 | -7.4 | -8.0 | -6.4 | -6.6 | | | | | | | | |
| L-86 | moderate | nh | -8.3 | -7.2 | -8.0 | -6.9 | -6.2 | | | | | | | | |
| LT-21 | moderate | nh | -8.6 | -6.8 | -7.1 | -8.2 | -8.8 | -8.2 | -8.1 | -6.0 | -6.2 | -7.3 | -8.0 | -6.9 | -6.1 |
| LTG-2 | moderate | nh | -7.8 | -6.8 | -6.9 | -7.3 | -7.9 | -8.0 | -7.4 | -6.2 | -6.5 | -8.1 | -8.4 | -6.9 | -6.8 |
| L-19 | moderate | nh | -8.3 | -6.6 | -7.1 | -6.7 | -8.3 | -8.1 | -7.9 | -6.2 | -6.4 | -7.6 | -7.9 | -6.6 | -6.1 |
| LT-24 | moderate | nh | -8.8 | -7.1 | -6.8 | -7.9 | -8.8 | -8.5 | -8.2 | -5.9 | -6.3 | -7.4 | -7.9 | -6.5 | -6.4 |
| LT-33 | moderate | nh | -8.0 | -6.1 | -7.2 | -7.0 | -7.9 | -7.9 | -7.7 | -5.8 | -5.9 | -7.1 | -8.0 | -6.1 | -5.5 |
| L-17 | moderate | nh | -8.0 | -6.6 | -7.4 | -8.3 | -8.1 | -7.9 | -7.8 | -6.1 | -6.3 | -7.4 | -8.0 | -6.5 | -6.0 |
| LT-34 | moderate | nh | -8.2 | -6.3 | -7.6 | -6.5 | -8.3 | -8.1 | -7.9 | -5.9 | -6.3 | -7.1 | -8.1 | -6.3 | -6.1 |
| LT-36 | moderate | nh | -8.2 | -6.3 | -7.1 | -6.2 | -7.8 | -8.1 | -7.7 | -5.8 | -6.0 | -7.0 | -8.1 | -6.7 | -5.9 |
| LT-50 | moderate | nh | -8.7 | -6.6 | -7.4 | -6.8 | -8.3 | -8.5 | -7.9 | -6.2 | -6.4 | -7.5 | -7.9 | -5.9 | -6.4 |
| LT-5 | moderate | nh | -8.5 | -6.5 | -7.1 | -8.0 | -8.1 | -7.9 | -8.0 | -5.8 | -6.2 | -7.0 | -7.5 | -6.1 | -5.6 |

Метод Байеса

STATISTICA - [Data: Docking TDAz_L17* (16v by 41c)]

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| | Docking | | | | | | | | | | | | | | | |
|-------|---------|-----------|----------|------|--------|--------|-------|------|------|------|-------------|-------------|------|------|-------|------|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| | SERT | SERT_h-nh | SERT_2-1 | NET | 5-HT3A | ADRA1A | CHRM1 | DRD1 | DRD2 | DAT | GABA-A GABA | GABA-A Benz | GAT1 | JAK3 | CAPN1 | CFD |
| LT-47 | -8.9 | h | 2 | -8.5 | -6.5 | -7.9 | -7.1 | -8.2 | -8.7 | -8.3 | -6.2 | -6.7 | -7.5 | -8.5 | -6.4 | -6.3 |
| LT-51 | -8.9 | h | 2 | -8.4 | -6.7 | -7.4 | -6.6 | -8.1 | -8.6 | -8.3 | -6.1 | -6.5 | -7.4 | -8.4 | -6.8 | -6.1 |
| LT-52 | -8.9 | h | 2 | -8.6 | -7.1 | -8.2 | -7.0 | -9.4 | -9.2 | -8.6 | -6.4 | -6.8 | -8.2 | -8.6 | -7.5 | -6.4 |
| L-91 | -8.7 | h | 2 | -8.6 | -6.9 | -6.9 | -8.3 | -9.2 | -8.7 | -8.9 | -6.1 | -6.4 | -7.5 | -8.2 | -7.0 | -6.3 |
| LT-13 | -8.7 | h | 2 | -8.6 | -7.2 | -8.2 | -7.2 | -9.0 | -8.9 | -8.7 | -6.3 | -6.5 | -7.5 | -8.2 | -6.4 | -5.8 |
| LT-23 | -8.7 | h | | | | | | | | | | | -7.6 | -8.1 | -7.0 | -6.0 |
| LT-48 | -8.7 | h | | | | | | | | | | | -7.6 | -8.0 | -6.6 | -6.1 |
| LT-46 | -8.6 | h | | | | | | | | | | | -7.4 | -8.2 | -6.2 | -6.0 |
| H-16 | -8.5 | h | | | | | | | | | | | -7.3 | -8.0 | -6.6 | -6.4 |
| H-88 | -8.5 | h | | | | | | | | | | | -7.2 | -7.9 | -6.8 | -6.3 |
| LT-22 | -8.5 | h | | | | | | | | | | | -7.5 | -8.2 | -6.8 | -6.5 |
| LT-49 | -8.5 | h | | | | | | | | | | | -7.6 | -8.0 | -6.3 | -6.3 |
| L-87 | -8.4 | h | | | | | | | | | | | -7.3 | -8.2 | -6.9 | -6.3 |
| LT-55 | -8.4 | h | | | | | | | | | | | -7.8 | -8.1 | -6.7 | -6.0 |
| LT-9 | -8.4 | h | | | | | | | | | | | -6.9 | -7.7 | -6.3 | -6.0 |
| L-20 | -8.3 | h | | | | | | | | | | | -7.4 | -8.1 | -6.6 | -6.1 |
| L-31 | -8.3 | h | | | | | | | | | | | -7.4 | -8.0 | -6.4 | -6.6 |
| L-86 | -8.3 | h | | | | | | | | | | | -7.2 | -8.0 | -6.9 | -6.2 |
| LT-21 | -8.3 | h | | | | | | | | | | | -7.3 | -8.0 | -6.9 | -6.1 |
| LTG-2 | -8.3 | h | | | | | | | | | | | -8.1 | -8.4 | -6.9 | -6.8 |
| L-19 | -8.2 | h | | | | | | | | | | | -7.6 | -7.9 | -6.6 | -6.1 |
| LT-24 | -8.2 | h | | | | | | | | | | | -7.4 | -7.9 | -6.5 | -6.4 |
| LT-33 | -8.2 | h | | | | | | | | | | | -7.1 | -8.0 | -6.1 | -5.5 |
| L-17 | -8.1 | nh | | | | | | | | | | | -7.4 | -8.0 | -6.5 | -6.0 |
| LT-34 | -8.1 | nh | | | | | | | | | | | -7.1 | -8.1 | -6.3 | -6.1 |
| LT-36 | -8.1 | nh | | | | | | | | | | | -7.0 | -8.1 | -6.7 | -5.9 |
| LT-50 | -8.1 | nh | 1 | -8.7 | -6.6 | -7.4 | -6.8 | -8.3 | -8.5 | -7.9 | -6.2 | -6.4 | -7.5 | -7.9 | -5.9 | -6.4 |
| LT-5 | -8.1 | nh | 1 | -8.5 | -6.5 | -7.1 | -8.0 | -8.1 | -7.9 | -8.0 | -5.8 | -6.2 | -7.0 | -7.5 | -6.1 | -5.6 |
| H-18 | -8.0 | nh | 1 | -8.6 | -6.7 | -6.8 | -6.6 | -8.2 | -8.0 | -8.2 | -6.1 | -6.3 | -7.4 | -7.9 | -6.3 | -6.4 |
| H-69 | -7.9 | nh | 1 | -8.2 | -6.5 | -7.1 | -6.5 | -8.0 | -8.1 | -8.1 | -5.9 | -6.2 | -7.4 | -7.8 | -6.3 | -6.4 |
| LT-30 | -7.9 | nh | 1 | -7.6 | -6.1 | -6.5 | -7.2 | -7.8 | -7.2 | -7.5 | -5.6 | -5.9 | -7.0 | -7.5 | -6.0 | -6.1 |
| LT-31 | -7.8 | nh | 1 | -7.8 | -6.1 | -6.1 | -5.9 | -7.8 | -7.2 | -7.3 | -5.6 | -5.9 | -7.1 | -7.6 | -6.1 | -5.7 |
| LT-35 | -7.8 | nh | 1 | -8.1 | -6.2 | -7.0 | -6.5 | -8.5 | -8.2 | -8.0 | -6.0 | -6.3 | -7.0 | -7.8 | -6.6 | -5.9 |
| LT-39 | -7.8 | nh | 1 | -8.2 | -6.2 | -6.7 | -6.3 | -8.4 | -8.1 | -8.2 | -5.7 | -6.0 | -7.3 | -7.6 | -6.2 | -5.8 |
| LT-29 | -7.7 | nh | 1 | -7.3 | -5.9 | -6.3 | -6.8 | -7.7 | -6.8 | -7.2 | -5.6 | -5.8 | -7.1 | -7.2 | -6.0 | -5.8 |
| LT-32 | -7.6 | nh | 1 | -7.7 | -6.2 | -6.0 | -6.7 | -7.6 | -7.3 | -7.6 | -5.3 | -5.7 | -7.0 | -7.4 | -6.1 | -5.8 |
| LT-38 | -7.6 | nh | 1 | -9.3 | -6.4 | -7.1 | -6.0 | -8.2 | -8.2 | -8.1 | -5.9 | -6.2 | -7.2 | -7.6 | -6.3 | -5.8 |
| LT-37 | -7.5 | nh | 1 | -9.3 | -6.3 | -7.0 | -6.2 | -8.3 | -8.1 | -8.1 | -5.9 | -6.2 | -7.1 | -7.7 | -6.5 | -5.7 |
| H-42 | -7.4 | nh | 1 | -7.4 | -6.0 | -6.2 | -6.4 | -7.5 | -7.3 | -7.0 | -5.4 | -5.6 | -7.0 | -7.3 | -6.3 | -5.8 |
| LT-53 | -7.4 | nh | 1 | -7.5 | -6.1 | -6.3 | -6.8 | -7.4 | -7.4 | -7.2 | -5.6 | -5.9 | -7.0 | -7.4 | -6.3 | -5.9 |

Machine Learning: Docking TDAz_L17

Quick

- Support Vector Machine
- Naive Bayes Classifiers**
- K-Nearest Neighbors

Naive Bayes for multiple classification tasks

OK

Cancel

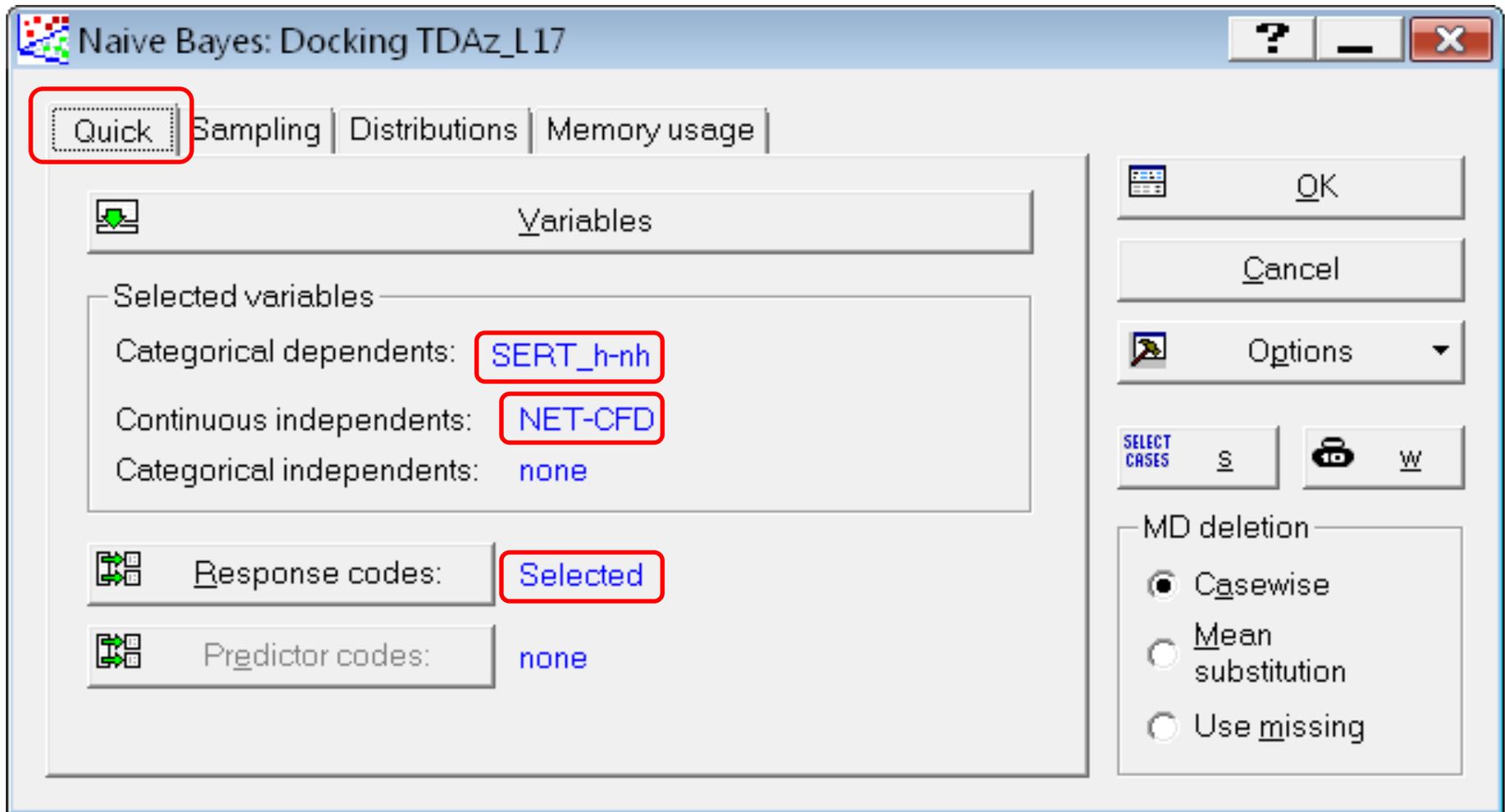
Options

Open Data

SELECT CASES

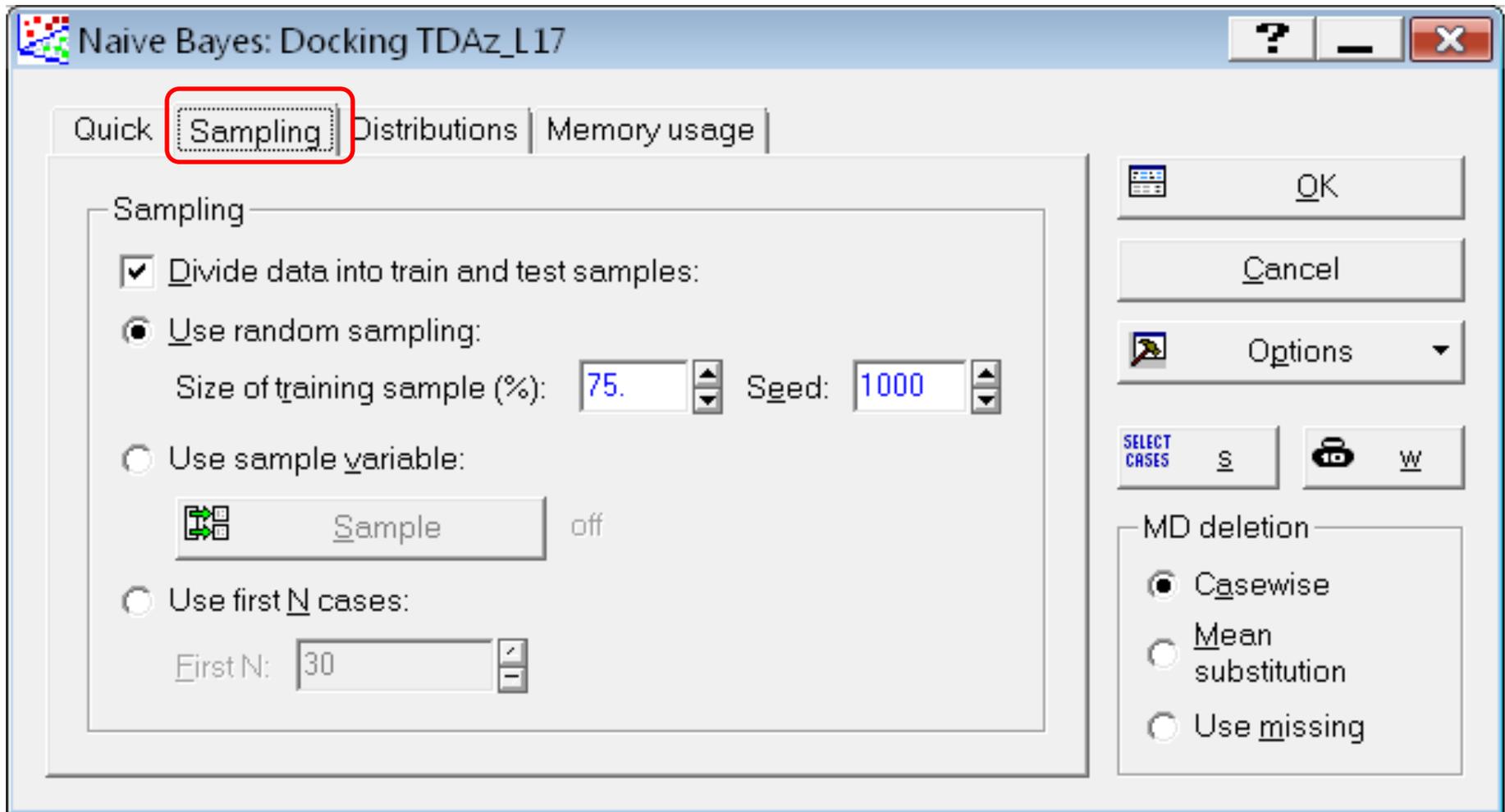
Метод Байеса

Выбор переменных



Метод Байеса

Выбор способа сэмплинга



Метод Байеса

Выбор функции распределения

Naive Bayes: Docking TDAz_L17

Quick | Sampling | **Distributions** | Memory usage

Threshold: .0001

Select distributions

| Independent | Type | Distribution |
|-------------|------------|--------------|
| NET | Continu... | Normal |
| 5-HT3A | Continu... | Normal |
| ADRA1A | Continu... | Normal |
| CHRM1 | Continu... | Normal |
| DRD1 | Continu... | Normal |
| DRD2 | Continu... | Normal |
| DAT | Continu... | Normal |
| GABA-A GABA | Continu... | Normal |

OK

Cancel

Options

SELECT CASES s

MD deletion

- Casewise
- Mean substitution
- Use missing

Метод Байеса

Общее описание модели

The screenshot shows the 'Naive Bayes Classifier Results: Docking TDAz_L17' window. The top section displays dataset information: 'Dataset Docking TDAz_L17:', 'Dependent: SERT_h-nh', 'Independents: NET, 5-HT3A, ADRA1A, CHRML, DRD1, DRD2, DAT, GABA-A GABA...', and 'Sample size = 30 (Train), 11 (Test), 41 (Overall)'. Below this, the 'Naive Bayes classifier results:' section shows 'Class labels: SERT_h-nh: h, nh'. The main interface has tabs for 'Quick', 'Plots', 'Prior', 'Posterior', and 'Custom predictions'. Under the 'Quick' tab, there are buttons for 'Summary', 'Model', and 'Descriptive statistics', with 'Model' and 'Descriptive statistics' highlighted by red boxes. The 'Predictions' section includes an 'Include' group with checkboxes for 'Independents', 'Dependents', 'Predictions', 'Accuracy', and 'Confidence'. At the bottom right, the 'Sample' section has radio buttons for 'Train', 'Test', and 'Overall', with 'Overall' selected and highlighted by a red box.

Naive Bayes Classifier Results: Docking TDAz_L17

Dataset Docking TDAz_L17:
Dependent: SERT_h-nh
Independents: NET, 5-HT3A, ADRA1A, CHRML, DRD1, DRD2, DAT, GABA-A GABA...
Sample size = 30 (Train), 11 (Test), 41 (Overall)

Naive Bayes classifier results:
Class labels:
SERT_h-nh: h, nh

Quick | Plots | Prior | Posterior | Custom predictions

Summary | Model | Descriptive statistics

Predictions

Include

Independents Dependents Predictions
 Accuracy Confidence

Predictions | Histograms | Save

Sample

Train
 Test
 Overall

Метод Байеса

Точность классификации

STATISTICA - [Workbook1* - Naive Bayes Results Dialog]

File View Statistics Data Mining Graphs Tools Workbook Window Help

Workbook1*

- Machine Learning (Docking TDAz_L17)
 - Naive Bayes Results Dialog**
 - Model summary (Naive Bayes Classifier), (Docking T
 - Naive Bayes model, SERT_h-nh (Docking TDAz_L17)
 - Classification summary (Naive Bayes Classifier), SERT
 - Confusion matrix (Naive Bayes Classifier), SERT_h-nh

| Model summary (Naive Bayes Classifier), (Docking T | |
|--|-------|
| | Value |
| Number of independents | 13 |
| Number of dependents | 1 |

| Class Name | Naive Bayes model, SERT_h-nh (Docking TDAz_L17) | | |
|------------|---|----------|------------------------|
| | Prior values | NET Mean | NET Standard deviation |
| h | 0.633333 | -8.43158 | 0.03894 |
| nh | 0.366667 | -8.04545 | 0.39072 |

| Class Name | Classification summary (Naive Bayes Classifier), SERT_h-nh | | | |
|------------|--|---------|-----------|------------|
| | Total | Correct | Incorrect | Correct(%) |
| h | 24 | 21 | 3 | 87.50000 |
| nh | 17 | 15 | 2 | 88.23529 |

| Class Predicted | Confusion matrix (Naive Bayes Classifier), SERT_h-nh | |
|-----------------|--|----|
| | Observed (rows) | h |
| h | 21 | 2 |
| nh | 3 | 15 |

Метод Байеса

Классификация нового объекта

The screenshot shows the 'Naive Bayes Classifier Results: Docking TDaz_L17' window. The top section displays dataset information: 'Dataset Docking TDaz_L17:', 'Dependent: SERT_h-nh', 'Independents: NET, 5-HT3A, ADRA1A, CHRML, DRD1, DRD2, DAT, GABA-A GABA...', and 'Sample size = 30 (Train), 11 (Test), 41 (Overall)'. Below this, the 'Naive Bayes classifier results:' section shows 'Class labels: SERT_h-nh: h, nh'. The interface includes a navigation bar with tabs for 'Quick', 'Plots', 'Prior', 'Posterior', and 'Custom predictions'. The 'Custom predictions' tab is active, showing a 'User defined case' input field and a 'Predictions' output field. On the right side, there are buttons for 'Summary', 'Cancel', 'Options', and 'Code generator'. At the bottom right, a 'Sample' section has radio buttons for 'Train', 'Test', and 'Overall', with 'Overall' selected.

Naive Bayes Classifier Results: Docking TDaz_L17

Dataset Docking TDaz_L17:
Dependent: SERT_h-nh
Independents: NET, 5-HT3A, ADRA1A, CHRML, DRD1, DRD2, DAT, GABA-A GABA...
Sample size = 30 (Train), 11 (Test), 41 (Overall)

Naive Bayes classifier results:
Class labels:
SERT_h-nh: h, nh

Quick | Plots | Prior | Posterior | Custom predictions

User defined case

Predictions

Summary

Cancel

Options

Code generator

Sample

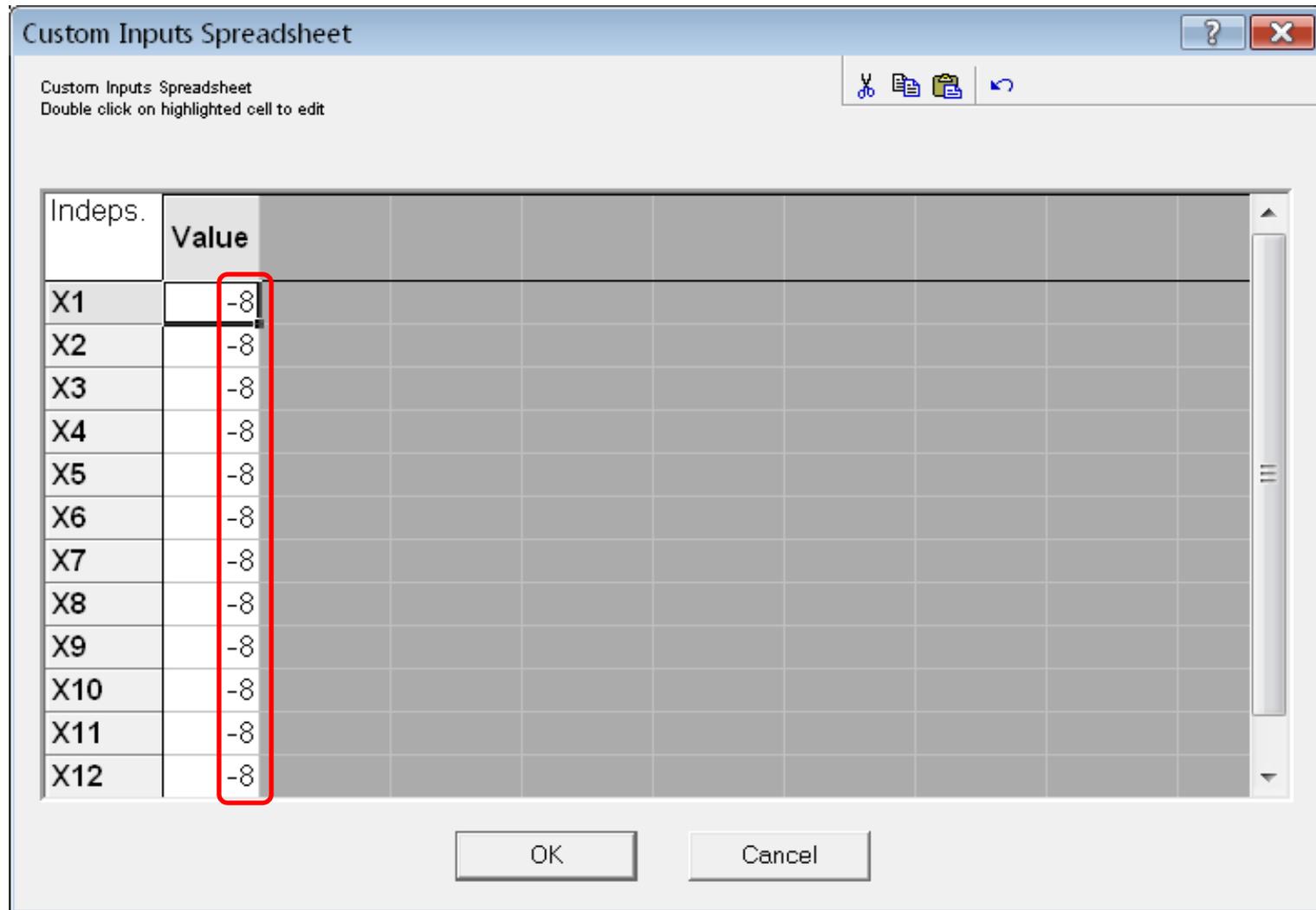
Train

Test

Overall

Метод Байеса

Задаем значения переменных



Метод Байеса

Выполняем прогноз

The screenshot shows the 'Naive Bayes Classifier Results: Docking TDz_L17' window. The main text area displays the following information:

```
Dataset Docking TDz_L17:  
Dependent: SERT_h-nh  
Independents: NET, 5-HT3A, ADRA1A, CHR11, DRD1, DRD2, DAT, GABA-A GABA...  
Sample size = 30 (Train), 11 (Test), 41 (Overall)
```

```
Naive Bayes classifier results:  
Class labels:  
SERT_h-nh: h, nh
```

Below the text area are several tabs: 'Quick', 'Plots', 'Prior', 'Posterior', and 'Custom predictions'. The 'Custom predictions' tab is active. In this tab, there are two rows of buttons:

- Row 1: A button with a question mark icon and the text 'User defined case'.
- Row 2: A button with a grid icon and the text 'Predictions', which is highlighted with a red rectangle.

On the right side of the window, there is a vertical toolbar with the following elements:

- 'Summary' button with a document icon.
- 'Cancel' button.
- 'Options' dropdown menu with a gear icon.
- 'Code generator' dropdown menu with a pencil icon.
- 'Sample' section with three radio buttons: 'Train', 'Test', and 'Overall' (which is selected).

Метод Байеса

Результат прогноза

STATISTICA - [Workbook1* - Custom predictions (Docking TDAz_L17)]

File Edit View Insert Format Statistics Data Mining Graphs Tools Data Workbook Window Help

GLM GLZ GRM PLS

Workbook1*

- Machine Learning (Docking TDAz_L17)
 - Naive Bayes Results Dialog
 - Model summary (Naive Bayes Classifier), (Docking TDAz_L17)
 - Naive Bayes model, SERT_h-nh (Docking TDAz_L17)
 - Classification summary (Naive Bayes Classifier), SERT_h-nh (Docking TDAz_L17)
 - Confusion matrix (Naive Bayes Classifier), SERT_h-nh (Docking TDAz_L17)
 - Custom predictions (Docking TDAz_L17)**

| Independent and dependent variables | Value |
|-------------------------------------|-----------|
| NET | -8.000000 |
| 5-HT3A | -8.000000 |
| ADRA1A | -8.000000 |
| CHRM1 | -8.000000 |
| DRD1 | -8.000000 |
| DRD2 | -8.000000 |
| DAT | -8.000000 |
| GABA-A GABA | -8.000000 |
| GABA-A Benz | -8.000000 |
| GAT1 | -8.000000 |
| JAK3 | -8.000000 |
| CAPN1 | -8.000000 |
| CFD | -8.000000 |
| SERT_h-nh | nh |

To be continued ...

