Machine Learning

2025 (ML-2025)

Lecture 3. Metrics and Metric Approach

by Alexei Kornaev, Dr. Sc., Assoc. Prof., Robotics and CV, Innopolis University
Researcher at the RC for AI, National RC for Oncology n.a. NN Blokhin

Agenda

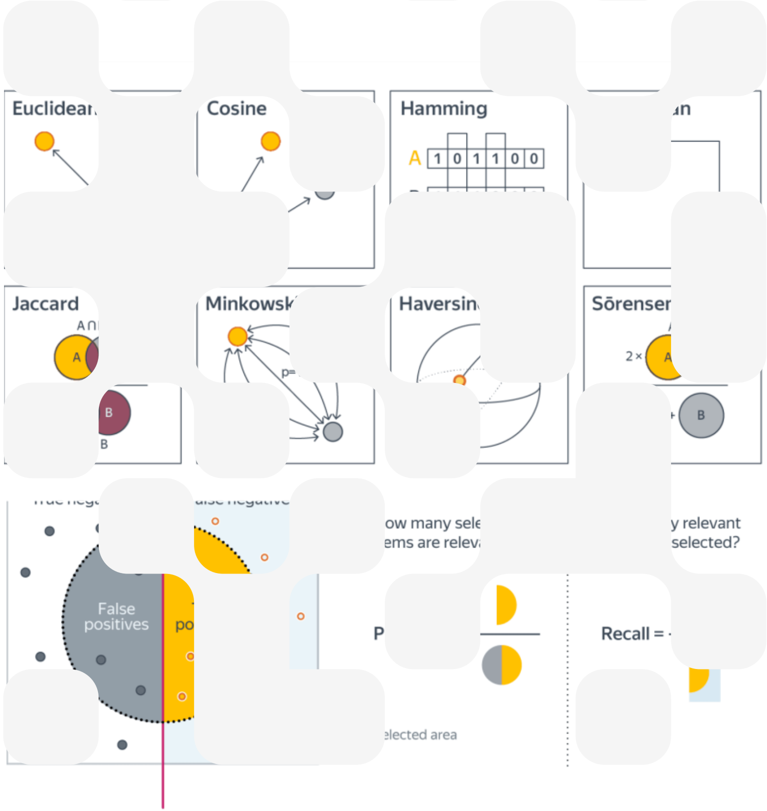
I. Quality metrics in ML

II. Data splitting, cross-validation

III. Regularization

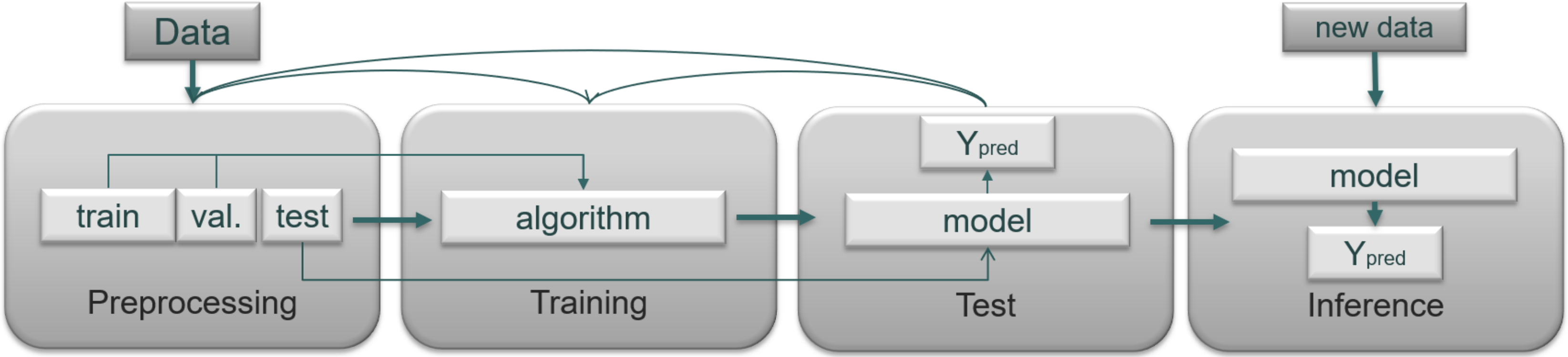
IV. Batches

V. Metric approach in ML: k-nearest neighbors

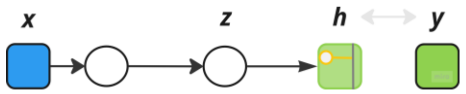


All models are wrong, but some are useful.
/George Box/

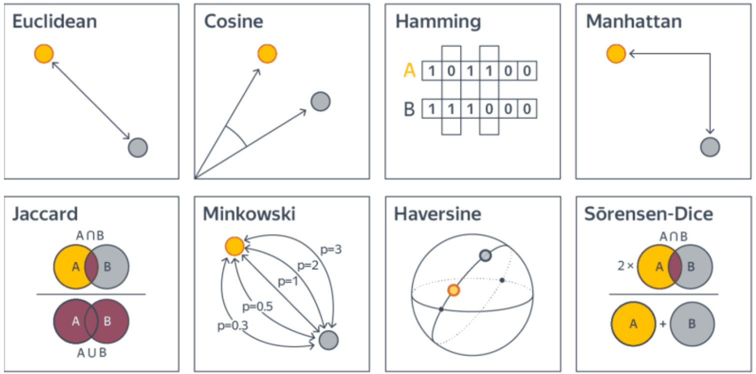
Flowchart for an ML model design

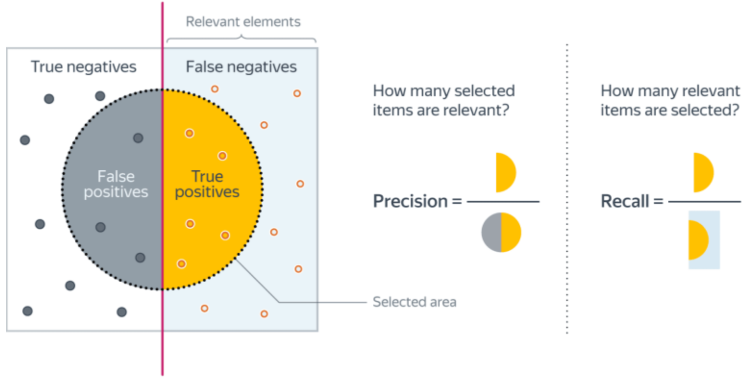


Metrics can be used both in learning (metric learning) and in estimating a model's quality



Model predicts output ***h*** given input ***x***

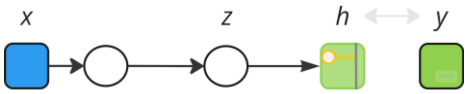




[Metrics from the Yandex Handbook]

[Classification metrics from the Yandex Handbook]

Metrics that estimate model's quality. Binary classification



Model predicts output *h* given input *x*

1. Accuracy: $acc(\boldsymbol{h}, \boldsymbol{y}) = \frac{1}{m}\sum_{i=1}^{m}(h^{(i)} == y^{(i)})$, or (and) error rate: $error\ rate = 1 - \mathrm{acc}(\boldsymbol{h}, \boldsymbol{y})$

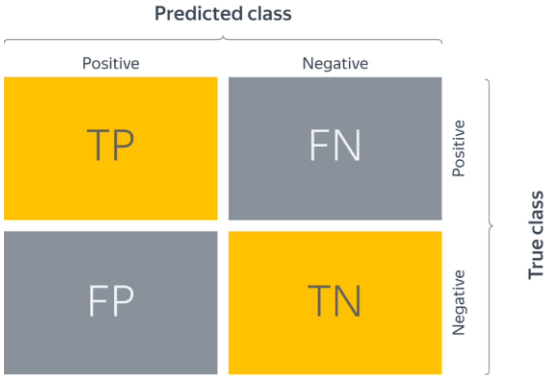
$$acc(\boldsymbol{h}, \boldsymbol{y}) = \frac{TP+TN}{TP+TN+FP+FN}.$$

$acc =$

Predicted	True
1	0
0	0
1	1
0	0
1	0
0	0
0	0
1	1
0	0
0	0

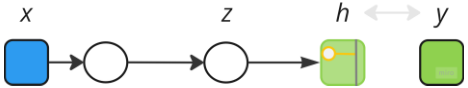
$acc =$

Predicted	True
0	1
0	0
0	0
0	0
0	1
0	0
0	0
0	0
0	0
0	0



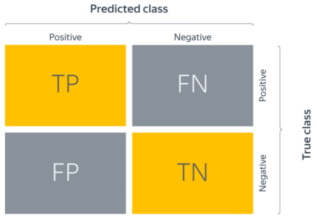
Confusion matrix

Metrics that estimate model's quality. Binary classification



Model predicts output *h* given input *x*

$$2.\ Precision = \frac{TP}{TP+FP},\ \ Recall = \frac{TP}{TP+FN},\ \ F_1 = \frac{Recall \cdot Precision}{Recall+Precision}.$$

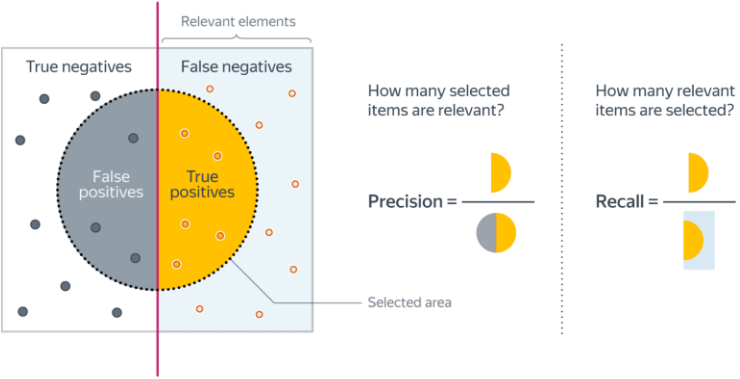


$pr =$ $re =$ $F_1 =$

Predicted	True
1	0
0	0
1	1
0	0
1	0
0	0
0	0
1	1
0	0
0	0

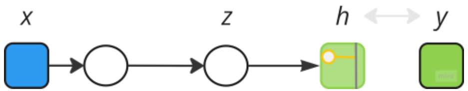
$pr =$ $re =$ $F_1 =$

Predicted	True
0	1
0	0
0	0
0	0
0	1
0	0
0	0
0	0
0	0
0	0



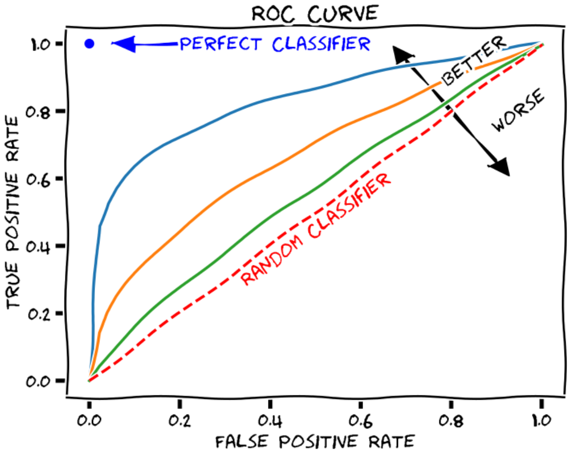
[Precision, recall, F1-score intuition]

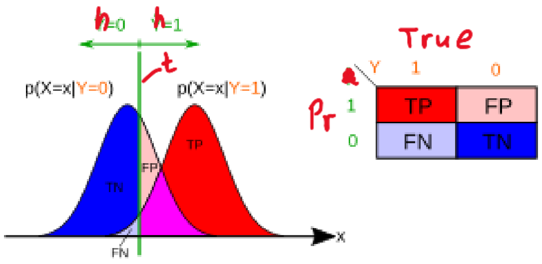
Metrics that estimate model's quality. Binary classification

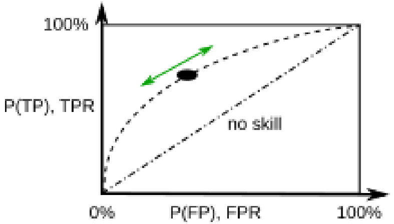


Model predicts output *h* given input *x*

1. True positive rate $TPR = Recall = \frac{TP}{TP+FN}$, false positive rate $FPR = \frac{FP}{FP+TN}$, Receiver operating characteristic (*ROC*), area under curve AUC.



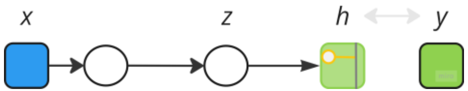




Overall, the optimization of precision and recall proceeds as follows:
- train the model on a loss function;
- obtain metric graphs depending on the threshold using real predictions on the validation set, by iterating over different thresholds from 0 to 1;
- select the desired combination of precision and recall.

[ROC curve intuition](#)

Metrics that estimate model's quality. Fitting



Model predicts output *h* given input *x*

1. Mean squared error (MSE):

$$MSE = \frac{1}{m}\sum_{i=1}^{m}\left(h^{(i)} - y^{(i)}\right)^2;$$

2. Mean absolute error (MAE):

$$MAE = \frac{1}{m}\sum_{i=1}^{m}\left|h^{(i)} - y^{(i)}\right|;$$

3. Root MSE (RMSE):

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(h^{(i)} - y^{(i)})^2}.$$

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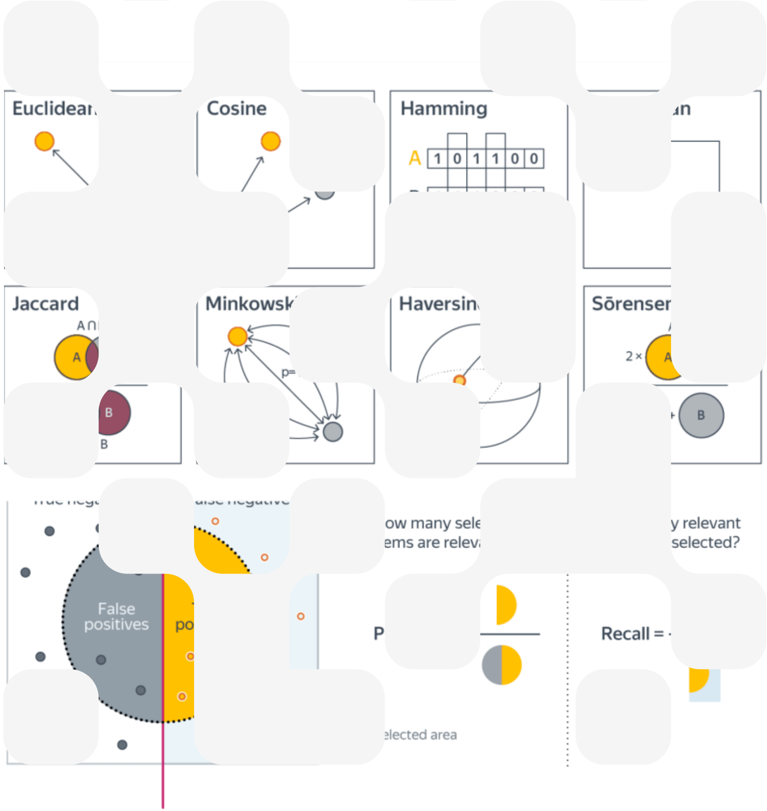

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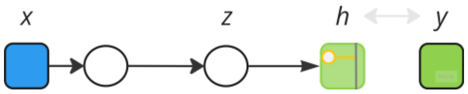
Overfitting intuition and data splitting

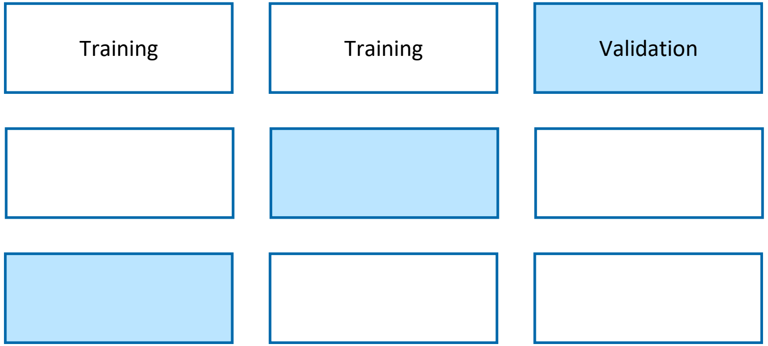


Model predicts output *h* given input *x*

Model *parameters* are determined during the solution of the ML problem, e.g. model weights. *Hyperparameters* are set by the user, usually not in a single way, and their values affect the values of the sought parameters.

Training data splitting by default: training set, validation set

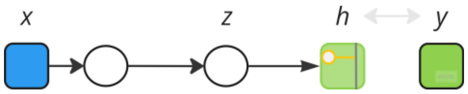
K-Fold splitting (normally used when the dataset is small)



Algorithm. The dataset is divided into *k* equal parts. Next, *k* iterations occur, during each of which one fold serves as the validation set, and the union of the remaining folds serves as the training set. The model is trained on *k-1* folds and tested on the remaining one. The final score of the model is obtained either by averaging the resulting test results or by measuring it on a held-out test set that did not participate in cross-validation.

Testing procedure: the accuracy of the selected trained model is checked on a new (test set)!!!

Overfitting intuition and data splitting



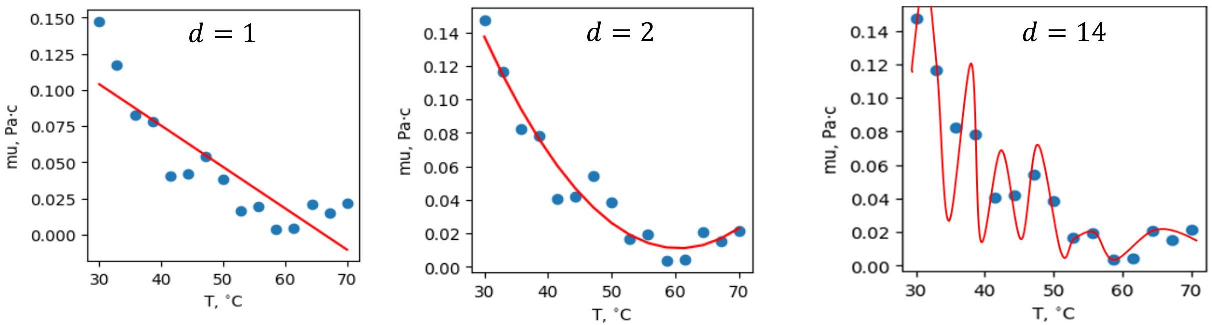
Model predicts output *h* given input *x*

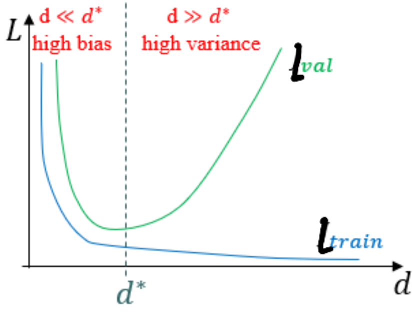
$$h = \theta_j x^j, (j = 0,..d)$$

$$\boxed{L = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h^{(i)} - y^{(i)}\right)^2\right] \Rightarrow \min.}$$

Model *parameters* are determined during the solution of the ML problem, e.g. model weights. *Hyperparameters* are set by the user, usually not in a single way, and their values affect the values of the sought parameters.

Training $\{(x_i, y_i)\}$	validation	test





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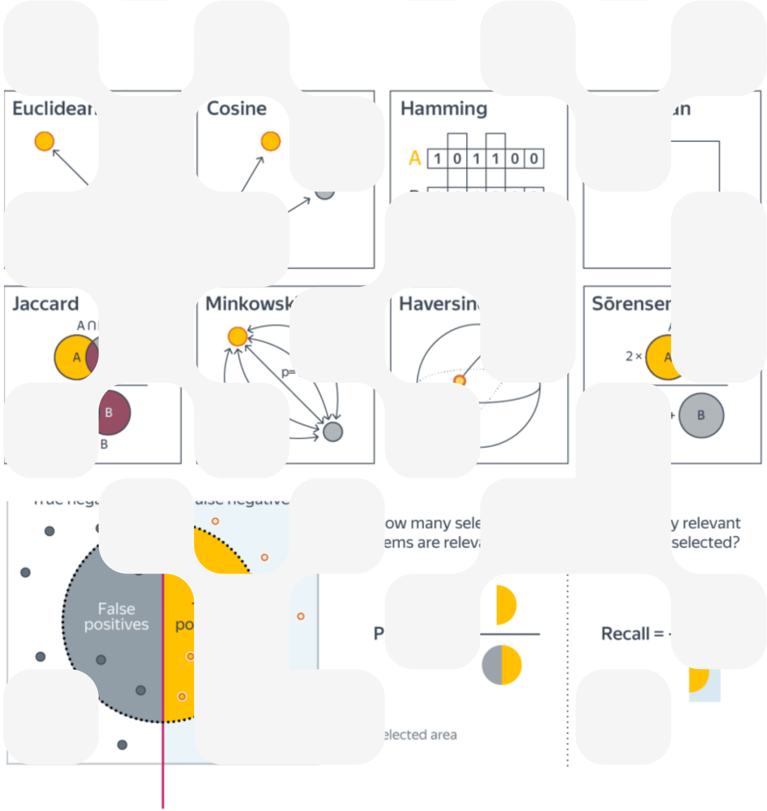

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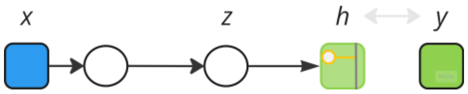
Overfitting intuition and regularization (L2)



Model predicts output *h* given input *x*

1. Feature Scaling
2. Learning Rate
3. Error and # of iterations
4. **Regularization (L2)**

Model *parameters* are determined during the solution of the ML problem. For example, in regression problems, the parameters are the components of the matrix of weights $\boldsymbol{\phi}$. *Hyperparameters* are set by the user, usually not in a single way, and their values affect the values of the sought parameters.

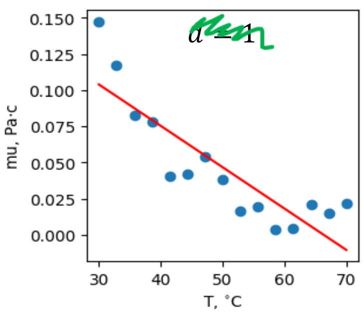
Training $\{(x_i, y_i)\}$	~~validation~~ val	test

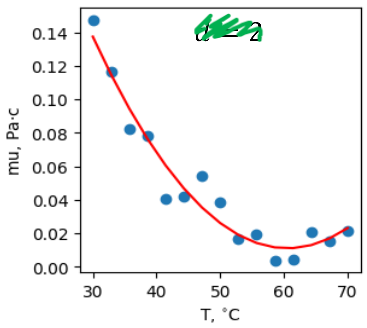
$\phi_0\ \phi_1 \ldots \phi_n$

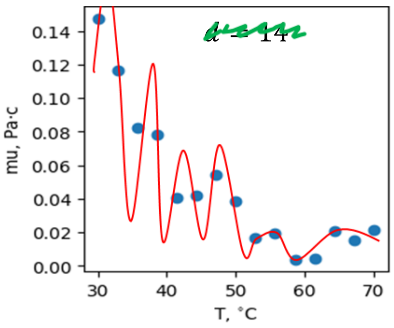
λ

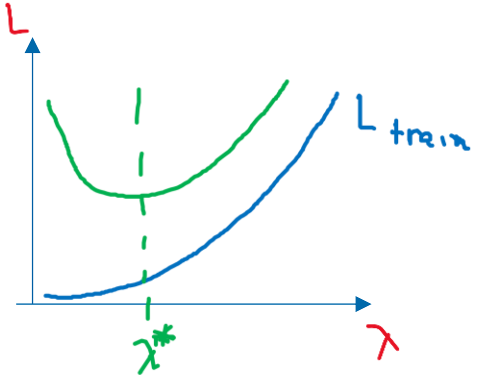
$$L = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h^{(i)} - y^{(i)}\right)^2 + \lambda \sum_{j=1}^{n} \phi_j^2\right] \Rightarrow \min.$$

$$h(x) = \theta_j x^j \quad ,(j = 0,..d)$$









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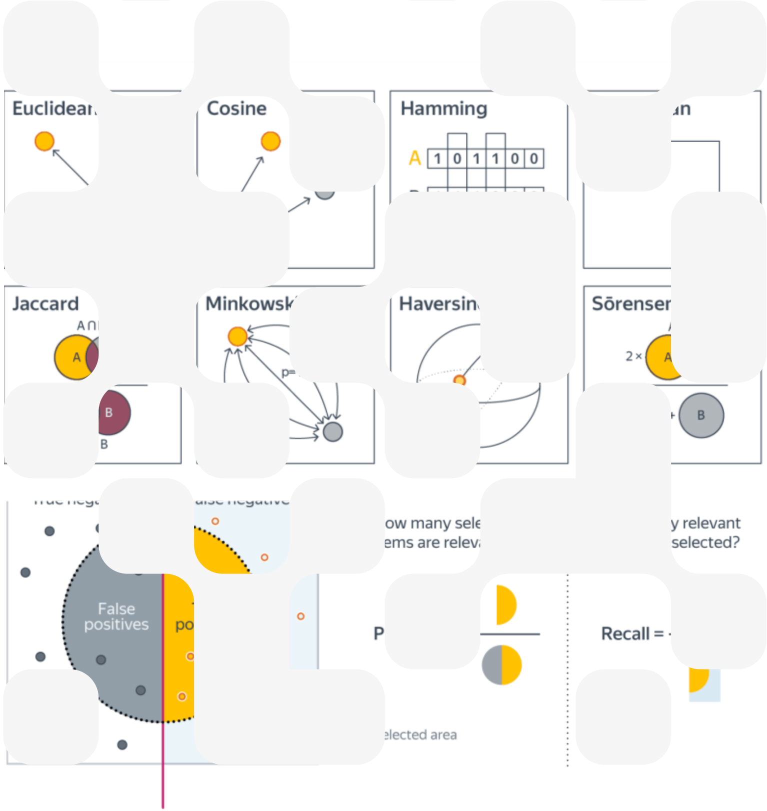

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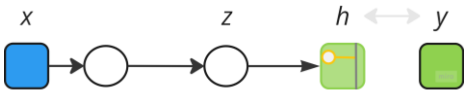

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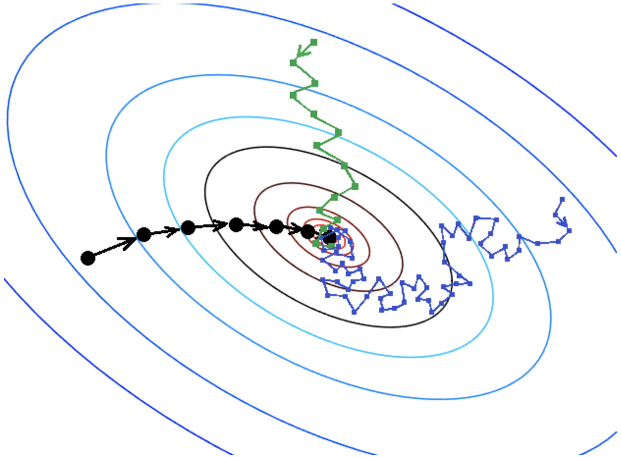

Batch GD
- **Slowest**
- **Perfect gradient**

Stochastic GD
- **Fastest**
- **Rough-estimate grad**

Mini-batch GD
- **Compromise**

https://dragonnotes.org/MachineLearning/Optimization

ML-2025. Metrics
by Alexei Kornaev

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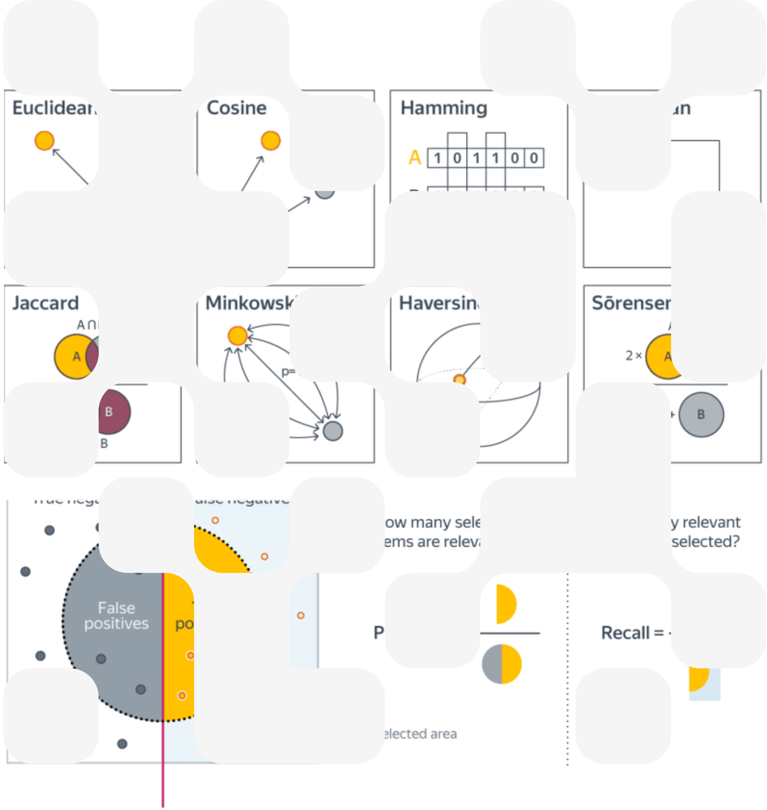

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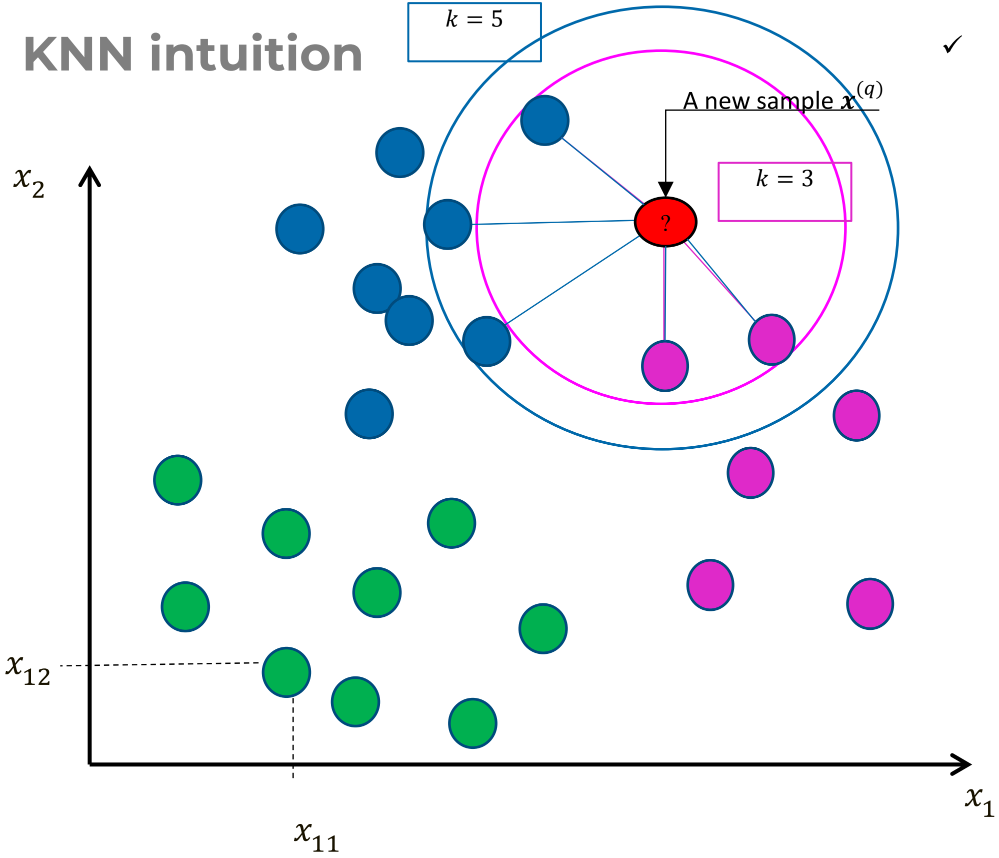
KNN intuition



✓ The compactness hypothesis: the assumption that similar objects are much more likely to be in the same class than in different ones.

Training:

- The training dataset is preserved $\{\boldsymbol{x}^{(i)}, y^{(i)}\}$;

Classification of a new object (sample):

- Compute the distance from all samples to the new sample $\boldsymbol{x}^{(q)}$;
- Sort the objects in ascending order of their distance to $\boldsymbol{x}^{(q)}$:

$$\rho\left(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(q)}\right) \leq \cdots \leq \rho\left(\boldsymbol{x}^{(j)}, \boldsymbol{x}^{(q)}\right) \leq \ldots \leq \rho\left(\boldsymbol{x}^{(r)}, \boldsymbol{x}^{(q)}\right)$$

- Select the first k samples (k nearest neighbors):

$$\{\boldsymbol{x}^{(i)}, \ldots, \boldsymbol{x}^{(j)}\}$$

- Assign the new sample the model class (most frequent class) among the KNN:

$$h\left(\boldsymbol{x}^{(q)}\right) = \underset{y_{cl} \in \mathbf{y}}{\operatorname{argmax}} \sum_{i=1}^{k} [y_i == y_{cl}].$$

Thank you for your attention!

a.kornaev@innopolis.ru, @avkornaev