Machine Learning

2024 (ML-2024)

Lecture 4. Quality metrics. Tips & tricks in ML: data splitting, cross-validation, regularization, batches

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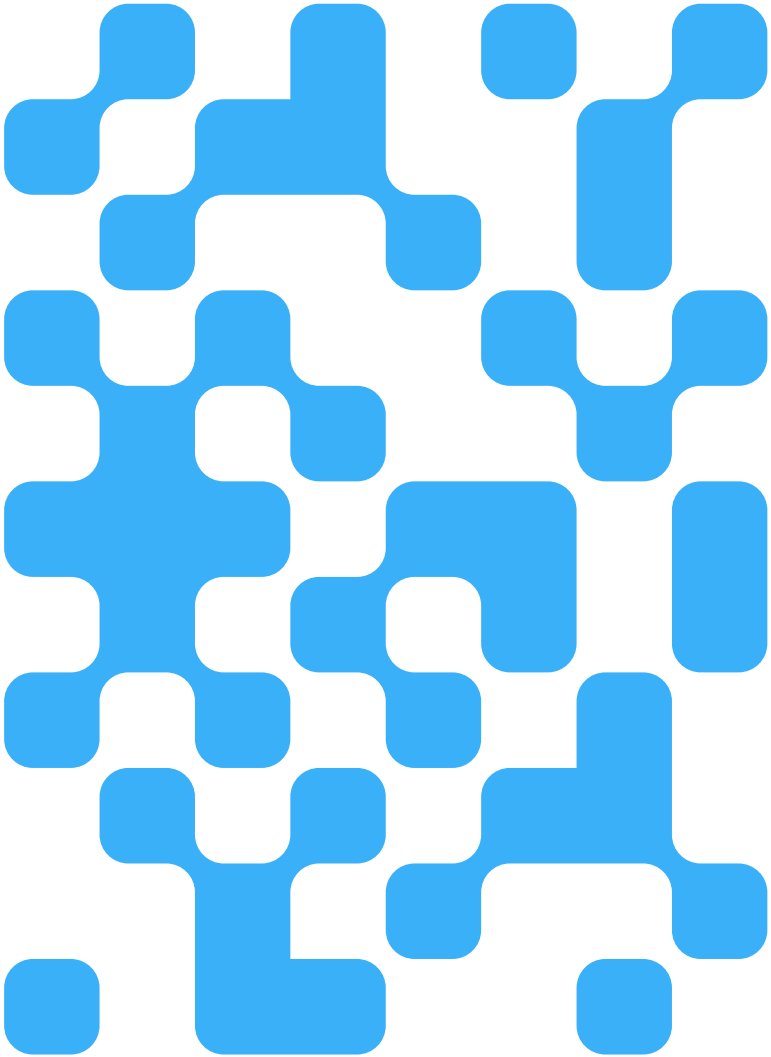


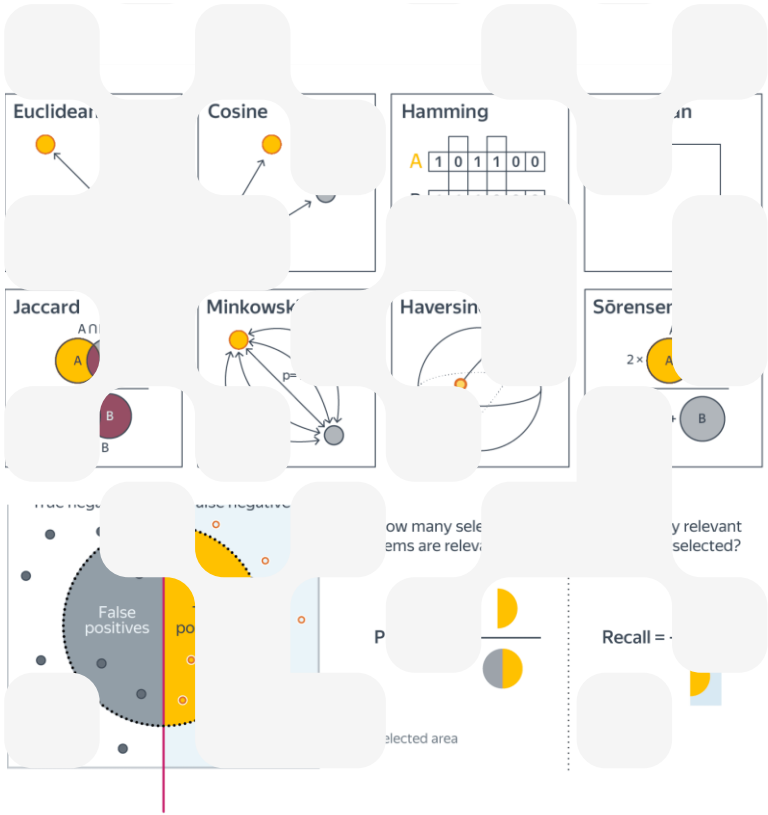
Agenda

I. Quality metrics in ML

II. Data splitting, cross-validation

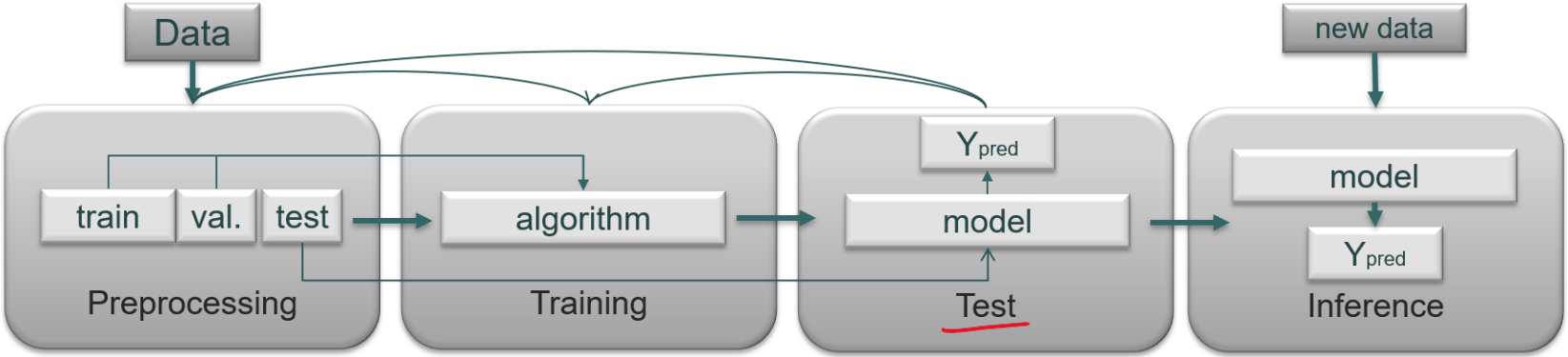
III. Regularization

IV. Batches



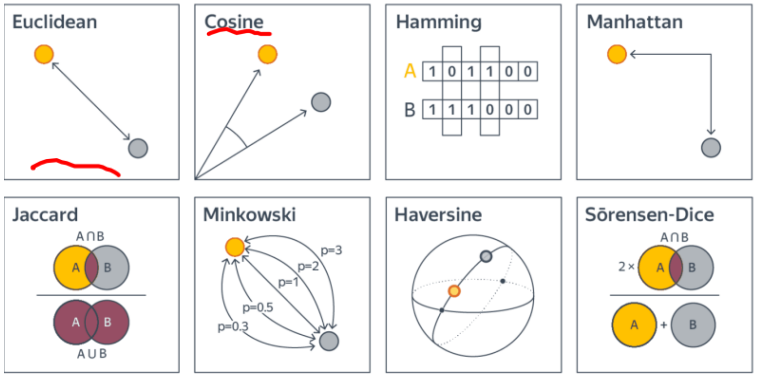
All models are wrong, but some are useful.
/George Box/

Flowchart for an ML model design

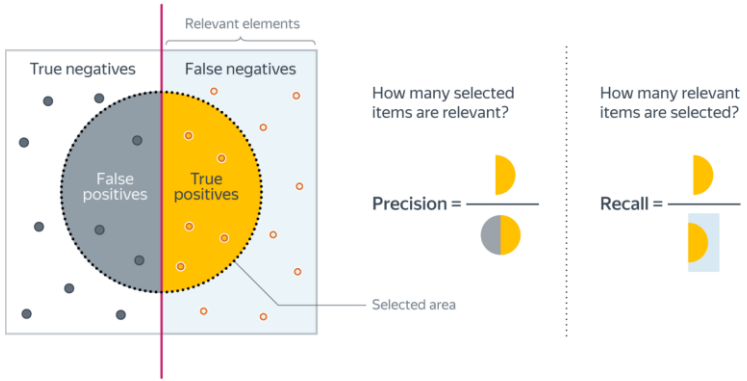


Metrics can be used both in learning (metric learning) and in estimating a model's quality

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

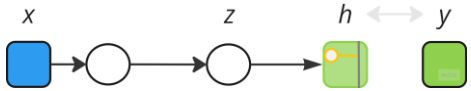


[Metrics from the Yandex Handbook]



[Classification metrics from the Yandex Handbook]

Metrics that estimate model's quality. Binary classification



Model predicts output *h* given input *x*

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

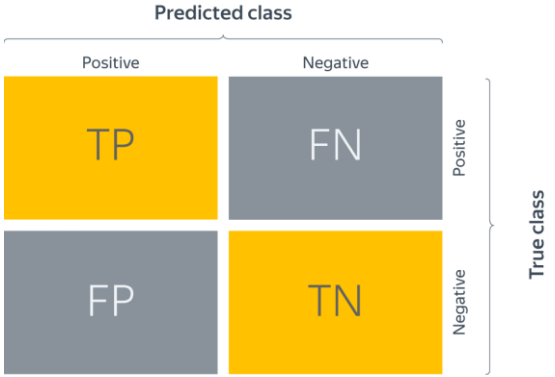
$$acc(\boldsymbol{h}, \boldsymbol{y}) = \frac{TP+TN}{TP+TN+FP+FN}.$$

$acc =$ 0.8

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

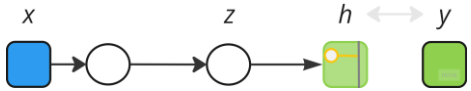
$acc =$ 0.8

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



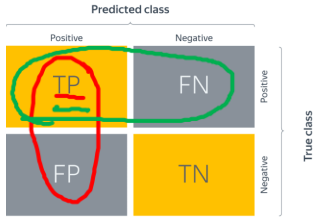
Confusion matrix

Metrics that estimate model's quality. Binary classification



Model predicts output *h* given input *x*

1 - rare class



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

F1 score

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

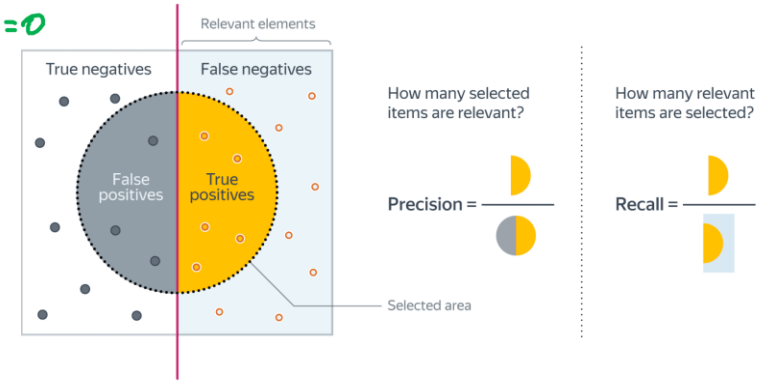
Predicted	True
1	0
0	0
1	1
0	0
1	0
0	0
0	0
1	1
0	0
0	0

FP

$pr = 0$ $re = 0$ $F_1 = 0$

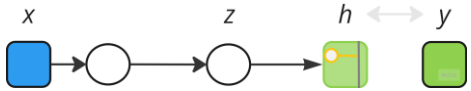
Predicted	True
0	1
0	0
0	0
0	0
0	1
0	0
0	0
0	0
0	0
0	0

TP=0



Precision, recall, F1-score intuition

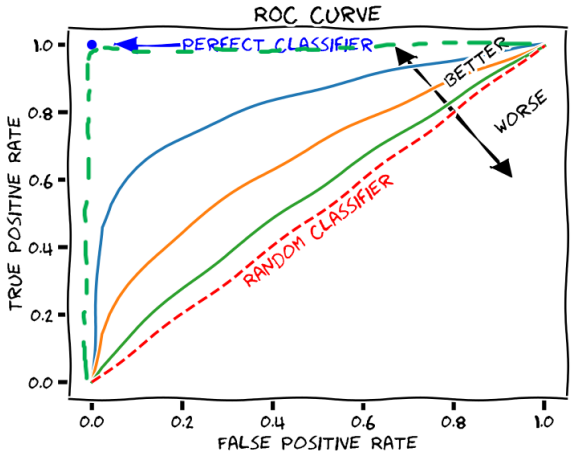
Metrics that estimate model's quality. Binary classification



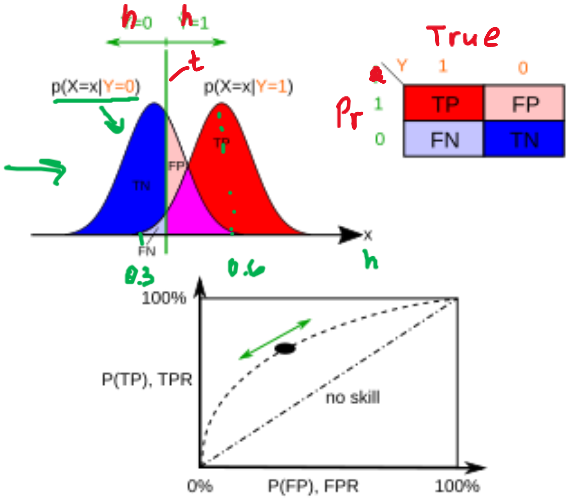
$h < t \to 0$; t is threshold - a tunable param.
$h \geq t \to 1$;

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.

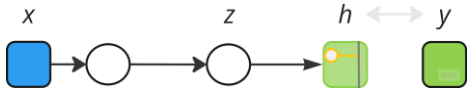


[ROC curve intuition]



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.

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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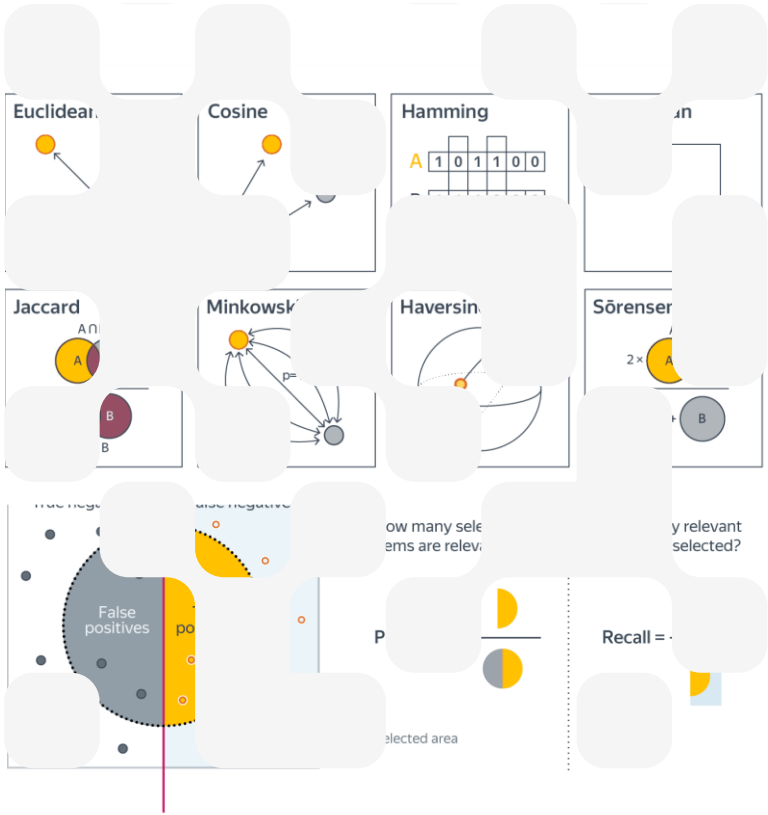
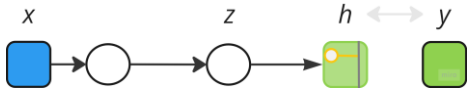


Overfitting intuition and data splitting

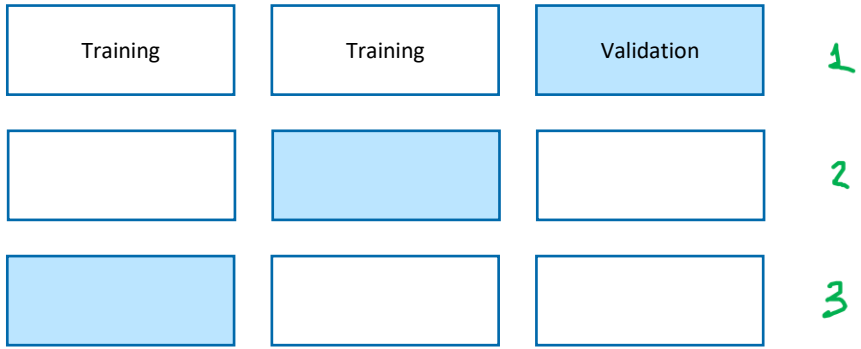


Model predicts output *h* given input *x*

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

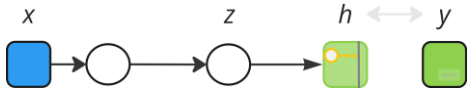
K-Fold splitting (normally used when the dataset is small)



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

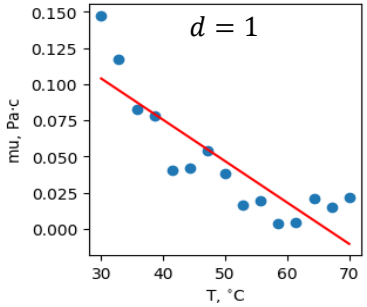


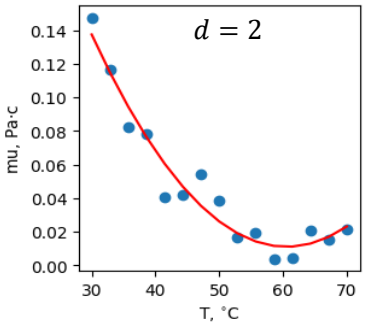
Model predicts output *h* given input *x*

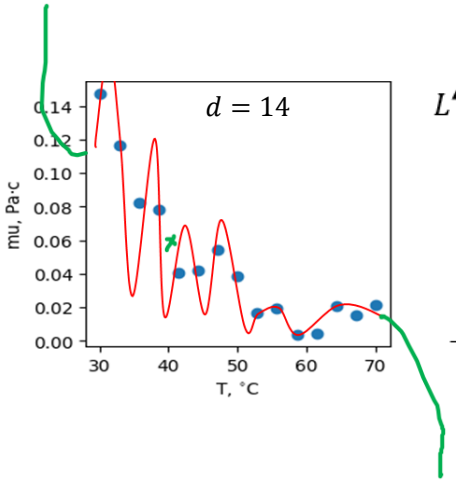
$$h = \theta_j x^j, (j = 0,..d)$$

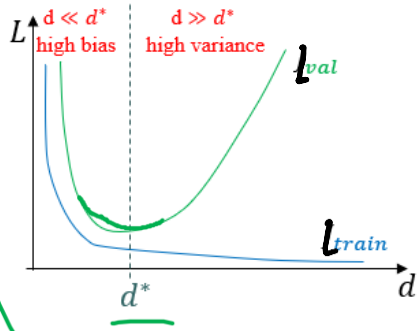
Model *parameters* are determined during the solution of the ML problem, e.g. model weights. *Hyperparameters* are set by the user, usually not in a single way, and their values affect the values of the sought parameters.

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









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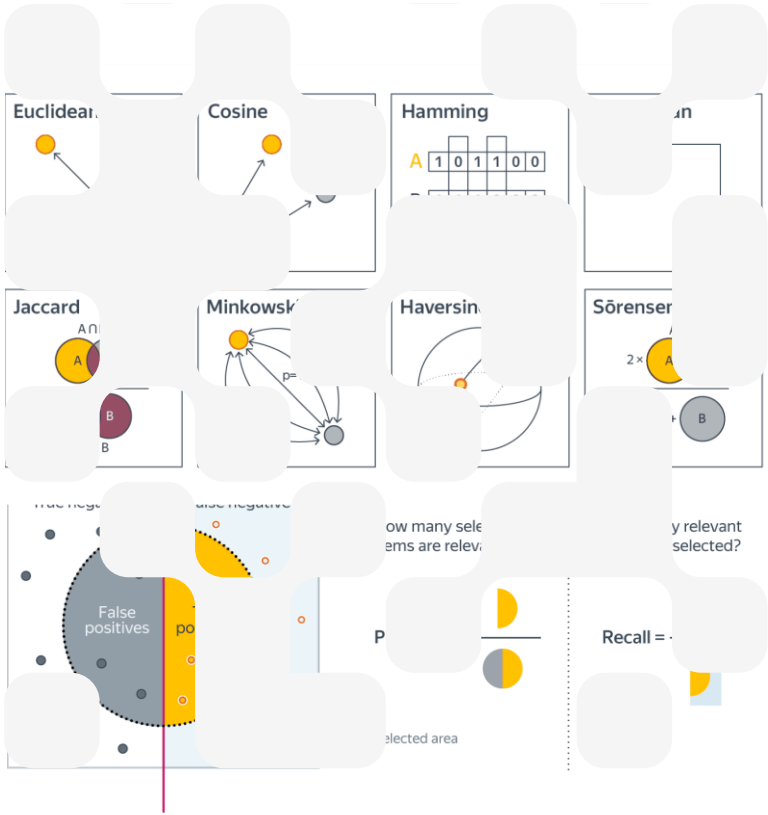

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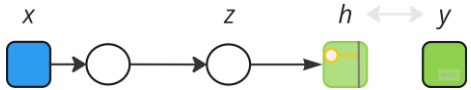
Overfitting intuition and regularization (L2)



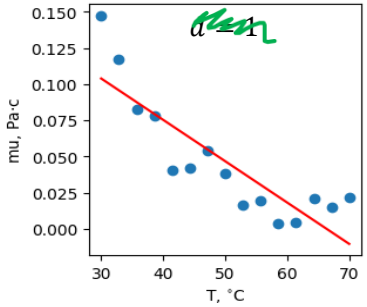
Model predicts output *h* given input *x*

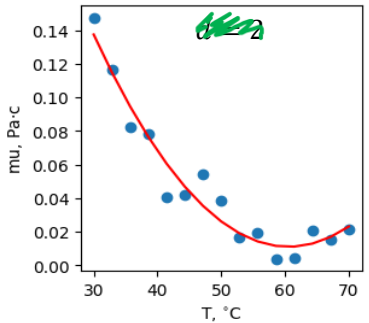
1. Feature Scaling
2. Learning Rate
3. Error and # of iterations
4. **Regularization (L2)**

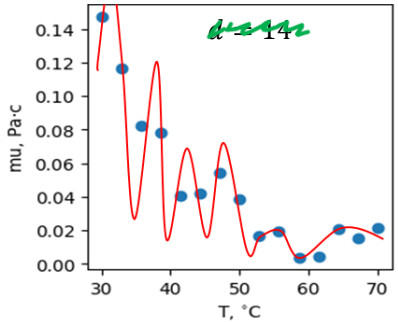
Model *parameters* are determined during the solution of the ML problem. For example, in regression problems, the parameters are the components of the matrix of weights $\boldsymbol{\phi}$. *Hyperparameters* are set by the user, usually not in a single way, and their values affect the values of the sought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

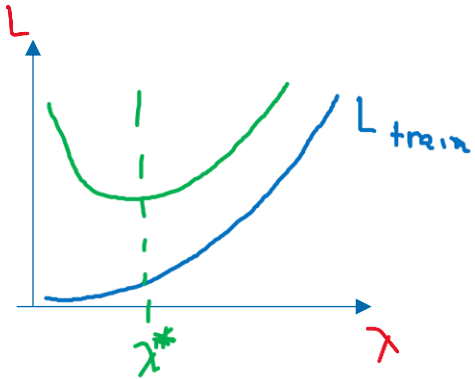
$$L = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h^{(i)} - y^{(i)}\right)^2 + \lambda \sum_{j=1}^{n} \phi_j^2\right] \Rightarrow \min.$$

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









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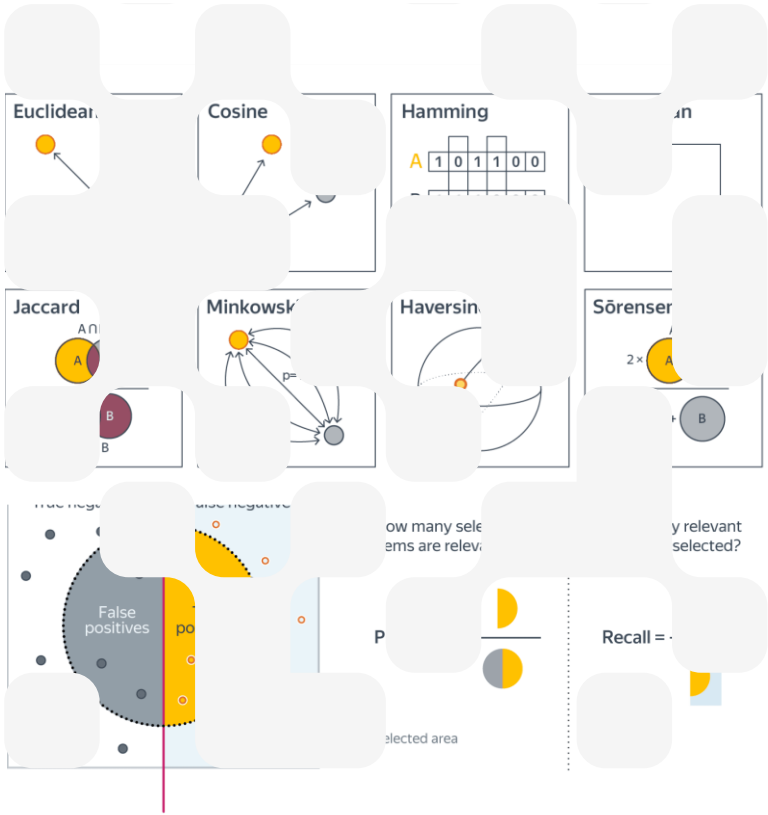

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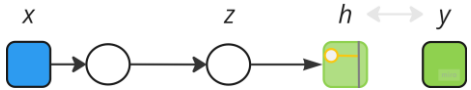

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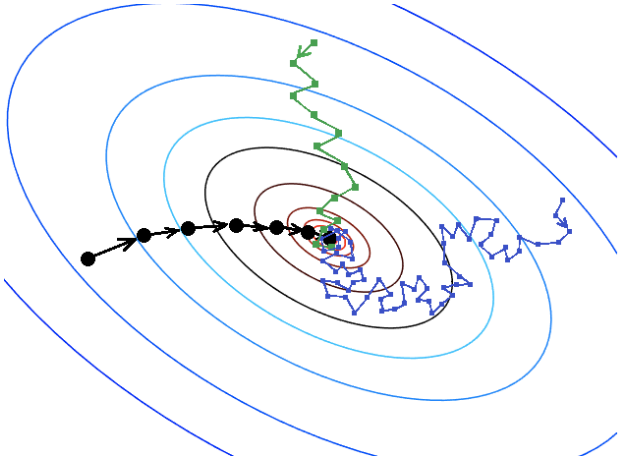

Batch GD
- Slowest
- Perfect gradient

Stochastic GD
- Fastest
- Rough-estimate grad

Mini-batch GD
- Compromise

https://dragonnotes.org/MachineLearning/Optimization

Thank you for your attention!

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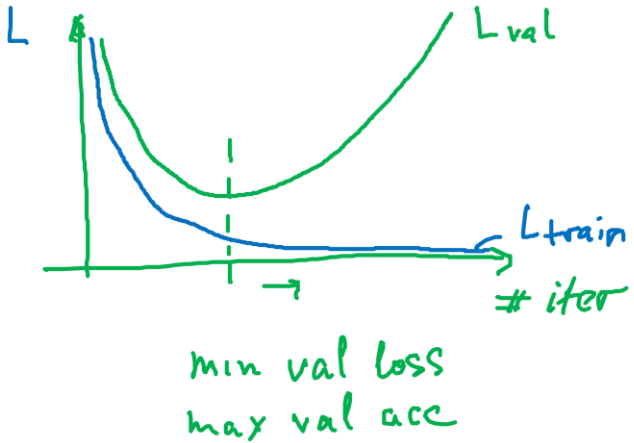

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