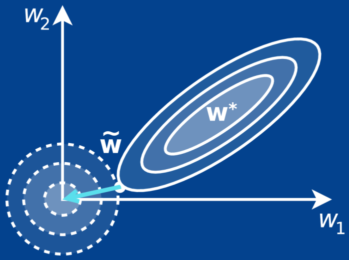
AARHUS UNIVERSITY
SCHOOL OF ENGINEERING

Lesson 8: Regularization, Optimization and Searching

CARSTEN EIE FRIGAARD

AUTUMN 2020



L08: Agenda

- ML Algorithm and Model Selection:
  k-fold Cross-Validation revisited,
  k-fold CV for Hyperparameter Tuning revisited.
- Regularization and Optimization:
  Regulizers,
  Exercise: `L09/regulizers.ipynb`
  Optimizers (no-exe).
- Searching:
  Gridsearch,
  Randomsearch,
  Exercise: `L09/gridsearch.ipynb`

ML Algorithm Selection and Model Selection

Manually Choosing an Algorithm and Tuning a Model..

- algorithm selection.

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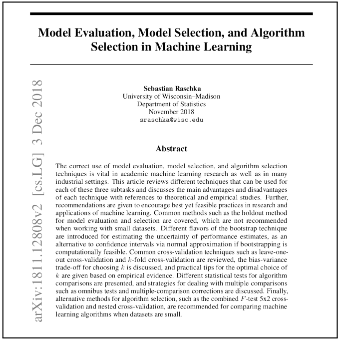


arXiv:1811.12808v2 [cs.LG] 3 Dec 2018

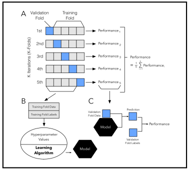
Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning

Sebastian Raschka
University of Wisconsin–Madison
Department of Statistics
November 2018
sraschka@wisc.edu

Abstract

The correct use of model evaluation, model selection, and algorithm selection techniques is vital in academic machine learning research as well as in many industrial settings. This article reviews different techniques that can be used for each of these three subtasks and discusses the main advantages and disadvantages of each technique with references to theoretical and empirical studies. Further, recommendations are given to encourage best yet feasible practices in research and applications of machine learning. Common methods such as the holdout method for model evaluation and selection are covered, which are not recommended when working with small datasets. Different flavors of the bootstrap technique are introduced for estimating the uncertainty of performance estimates, as an alternative to confidence intervals via normal approximation if bootstrapping is computationally feasible. Common cross-validation techniques such as leave-one-out cross-validation and k-fold cross-validation are reviewed, the bias-variance trade-off for choosing k is discussed, and practical tips for the optimal choice of k are given based on empirical evidence. Different statistical tests for algorithm comparisons are presented, and strategies for dealing with multiple comparisons such as omnibus tests and multiple-comparison corrections are discussed. Finally, alternative methods for algorithm selection, such as the combined F-test 5x2 cross-validation and nested cross-validation, are recommended for comparing machine learning algorithms when datasets are small.

"Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning",
Sebastian Raschka, 2018.



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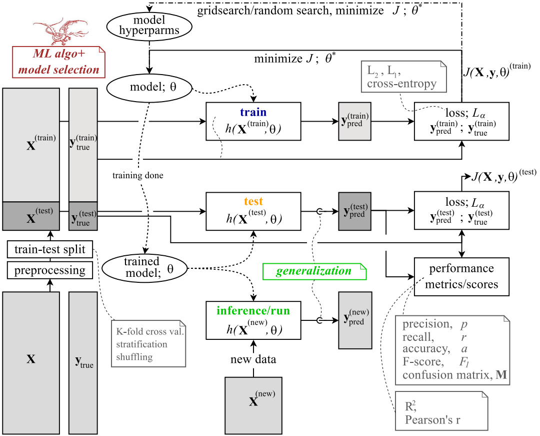

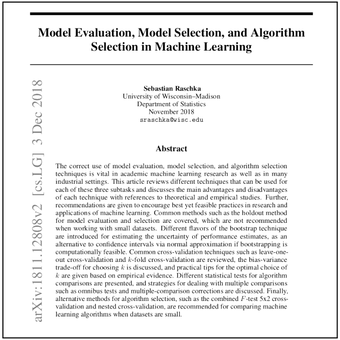

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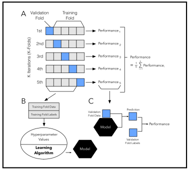

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  - the performance metric `score` function,
  - how do you evaluate **generalization** performance?
  - holdout method (train-test split) and k-fold CV,
  - three-way split (train-validate-test split)..

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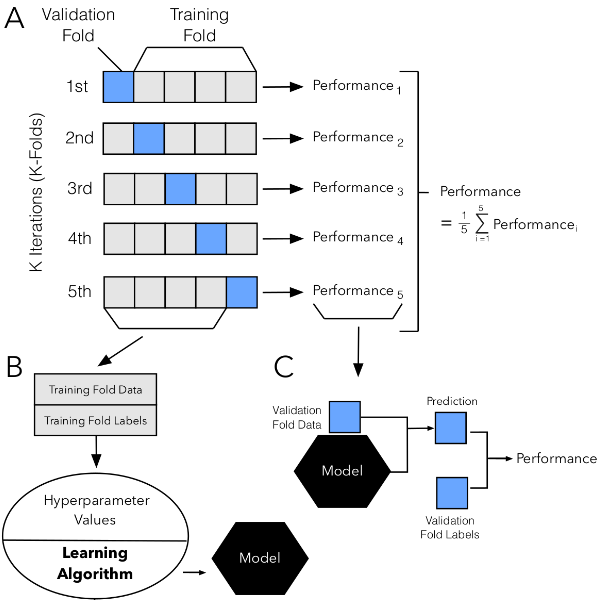
- re-iteration and re-selection!

NOTE: Model selection: ∼ selection the best capacity/hyperparameter for a given model—NOT choosing the ML algo/model itself!

Model Evaluation

k-fold Cross-Validation Procedure, for *k*=5..



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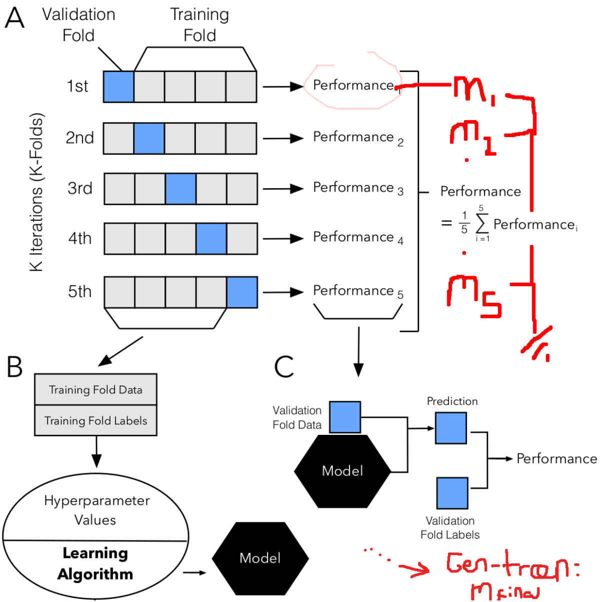
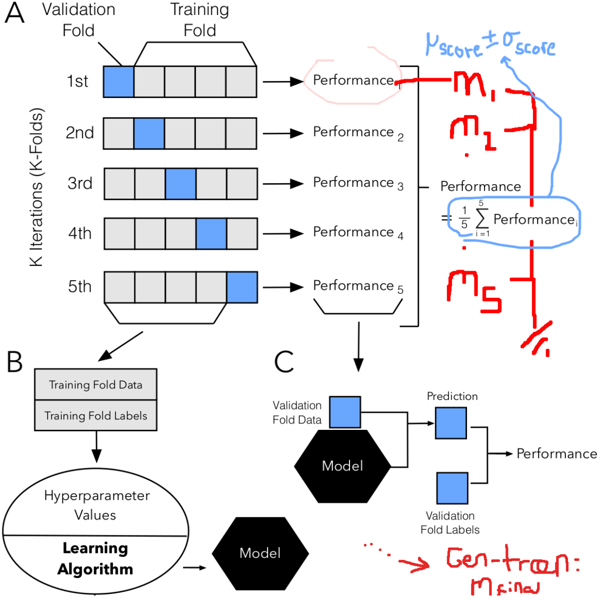
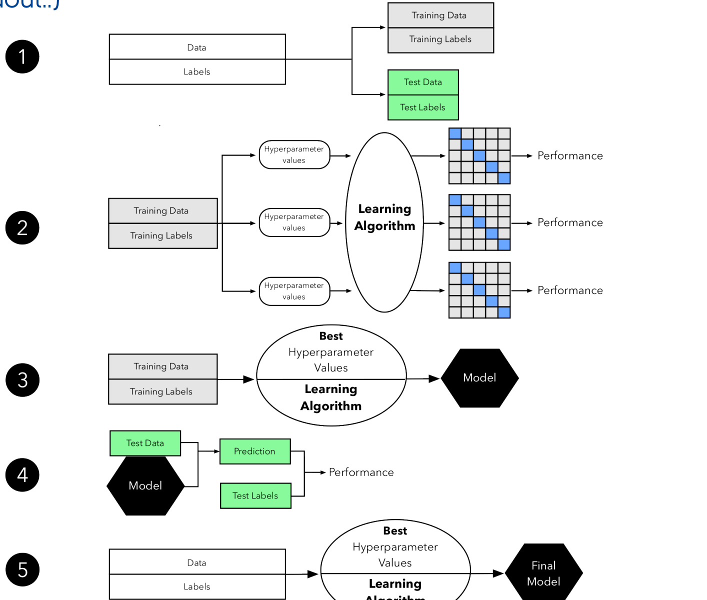



A
Validation Fold
Training Fold
1st
2nd
3rd
4th
5th
K Iterations (K-Folds)
Performance 1
Performance 2
Performance 3
Performance 4
Performance 5
Performance
$= \frac{1}{5}\sum_{i=1}^{5} \text{Performance}_i$
$\mu_{score} \pm \sigma_{score}$
m_1
m_5
B
Training Fold Data
Training Fold Labels
Hyperparameter Values
Learning Algorithm
Model
C
Validation Fold Data
Prediction
Model
Performance
Validation Fold Labels
Gen-tran:
m_{final}

Model Evaluation and Selection

k-fold Cross-Validation for Hyperparameter Tuning (Somewhat Similar to Treeway Holdout..)



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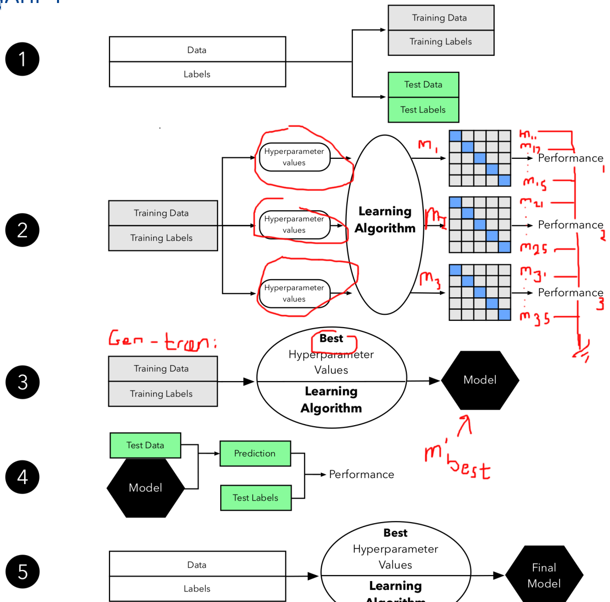

Regularization

Adding a Penalty to the Cost Function

For a linear regressor, our cost function was

$$J(\mathbf{X}, \mathbf{y}; \mathbf{w}) = ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \propto \mathrm{MSE}(\mathbf{X}, \mathbf{y}; \mathbf{w})$$

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The effect of the added penalty is to:

- put a **contraint** on the norm of the weights, $\mathbf{w}$, disallowing 'em to grow wildely,
- leading to **reduced overfitting**, disabling the model to learn the background noise in the data.

$\mathcal{L}_2$ Regularization

Ridge Penalization

Aka Weight Decay, aka Tikhonov regularization

$$\begin{aligned} \Omega(\mathbf{w}) &= ||\mathbf{w}||_2^2 = \mathbf{w}^\top \mathbf{w} \\ \tilde{J}_{\text{ridge}}(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= J(\mathbf{X}, \mathbf{y}; \mathbf{w}) + \alpha \mathbf{w}^\top \mathbf{w} \end{aligned}$$

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with $\mathbf{w} = [w_1 \ w_2 \ \cdots \ w_n]^\top$ without the bias element w_0 in the regulizer term, Ω, and recalling the Euclidiean norm

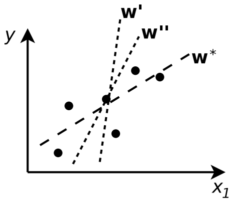
$$\mathcal{L}_2^2 : ||\mathbf{x}||_2^2 = \mathbf{x}^\top \mathbf{x}$$

NOTE: ..and give-or-take some additional $1/2$ or $1/n$ constant, that we do not care about.

$\mathcal{L}_2$ Regularization

Ridge Penalization

A graphical view for a linear regressor



1D featurespace

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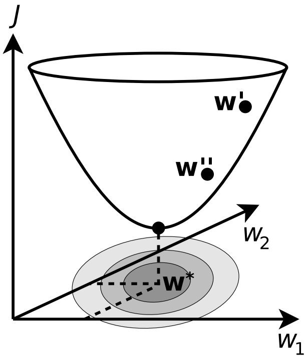
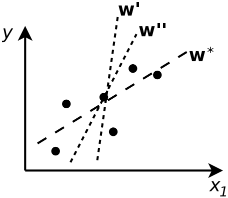


3D: ideal convex loss in $J - \mathbf{w}$ space.



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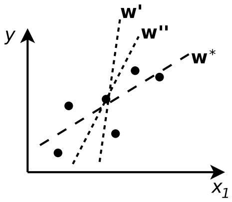

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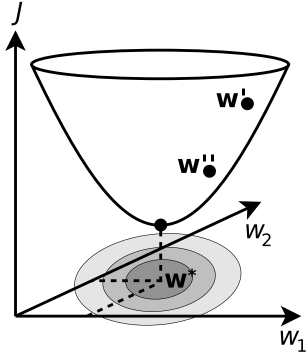

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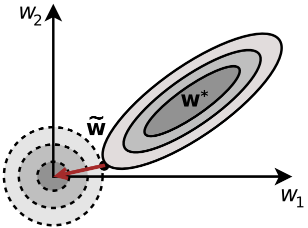

2D: flat $w_2 - w_1$ view with some feature scaling.

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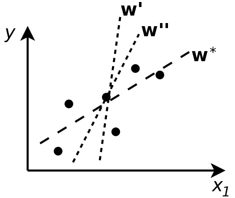

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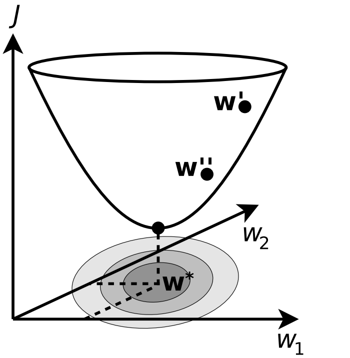

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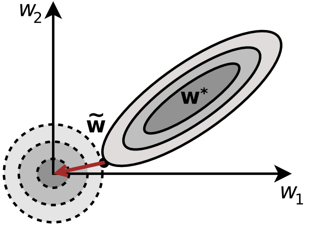

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The tug-of-war: what happens with $\tilde{\mathbf{w}}$,
if $\mathbf{w}^*$ is far from the origin $[w_1, w_2] = (0, 0)$?

$\mathcal{L}_1$ Regularization

Lasso penalization

Now, just replace the $\mathcal{L}_2$ with $\mathcal{L}_1$ and we have the Lasso regularizer

$$\begin{aligned} \Omega(\mathbf{w}) &= ||\mathbf{w}||_1 \\ \tilde{J}_{\text{lasso}}(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= J(\mathbf{X}, \mathbf{y}; \mathbf{w}) + \alpha ||\mathbf{w}||_1 \end{aligned}$$

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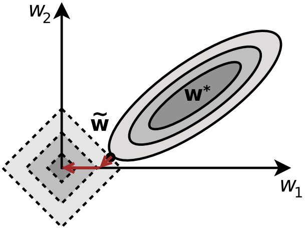
with the Manhattan norm

$$\mathcal{L}_1 : ||\mathbf{x}||_1 = \sum_{i=1}^{n} \text{abs}(x_i)$$

and the $\mathcal{L}_1$ penalty tends to drive weights to zero:

- automatic feature selection,
- outputs a sparce model,
- i.e few nonzero w's.



$\mathcal{L}_1$ and $\mathcal{L}_2$ Regularization

Elastic-net Penalization

And finally a combination of the two: an Elastic-net regularizer

$$\begin{aligned}
\Omega(\mathbf{w}) &= \beta||\mathbf{w}||_1 + (1-\beta)||\mathbf{w}||_2^2 \\
\tilde{J}_{\text{elastic}}(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= J(\mathbf{X}, \mathbf{y}; \mathbf{w}) + \alpha\left(\beta||\mathbf{w}||_1 + (1-\beta)||\mathbf{w}||_2^2\right)
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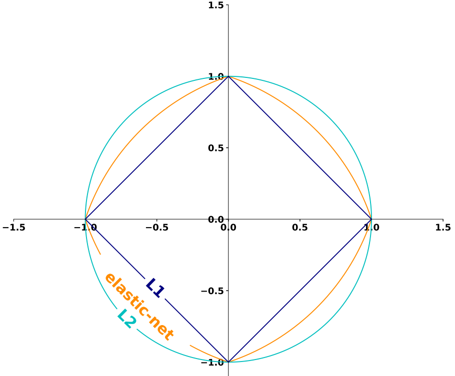

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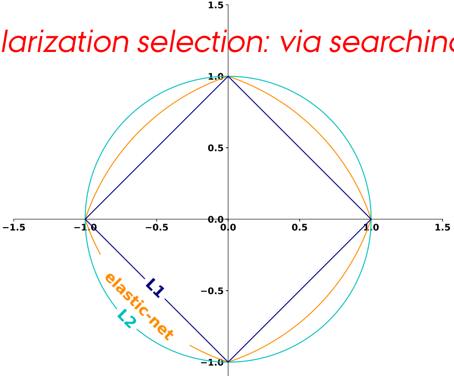
Regularization selection: via searching..



Optimizers

Momentum Optimization

Normal GD algo

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} J$$

but now with added (physical) momentum

$$\begin{aligned} \mathbf{m} &\leftarrow \beta \mathbf{m} - \eta \nabla_{\mathbf{w}} J \\ \mathbf{w} &\leftarrow \mathbf{w} + \mathbf{m} \end{aligned}$$

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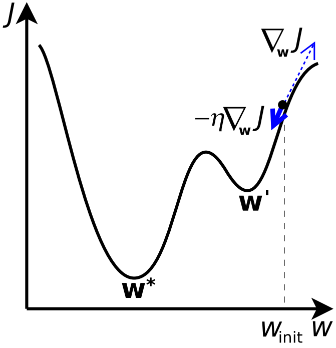

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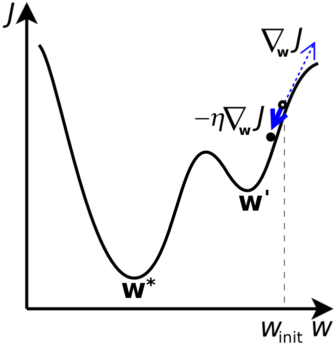

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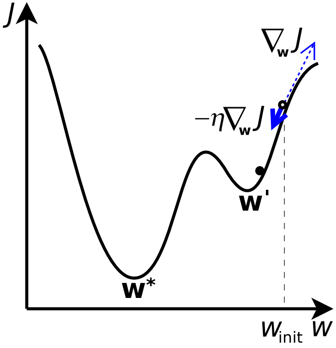

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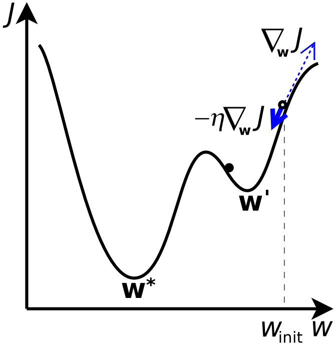

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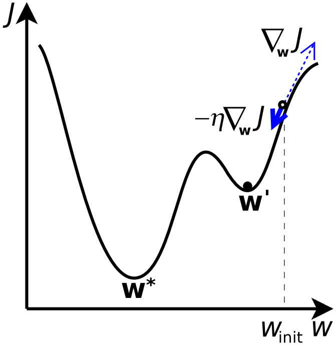

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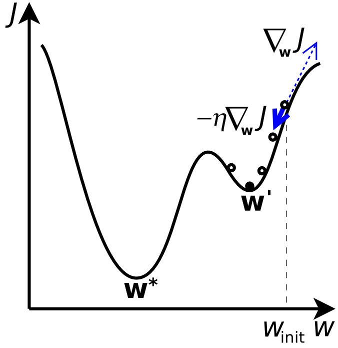

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Momentum Optimization

Normal GD algo

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} J$$

but now with added (physical) momentum

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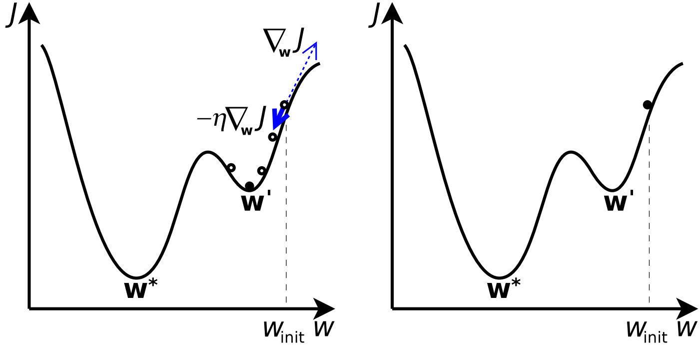

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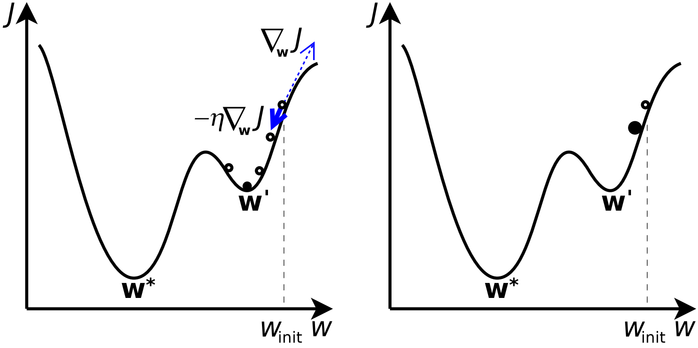

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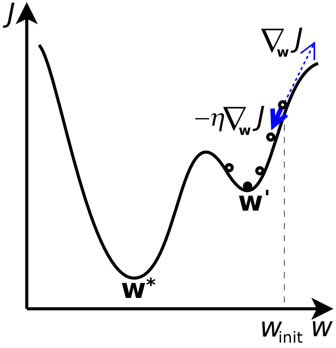

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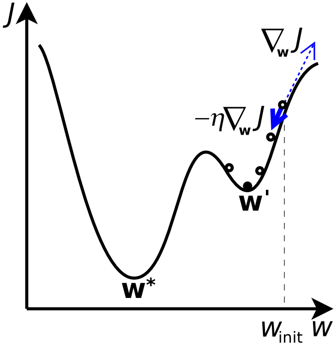

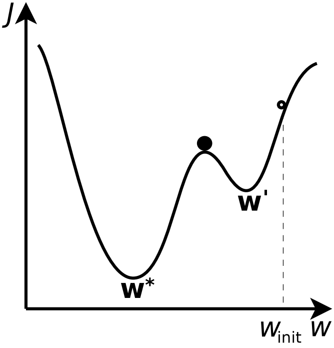

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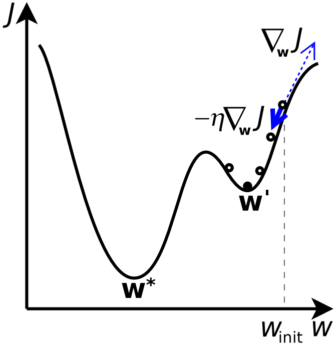

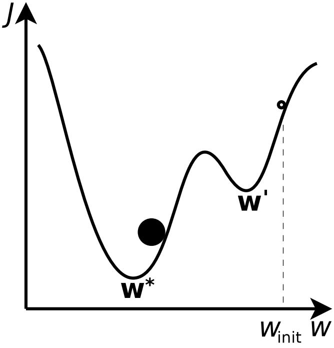

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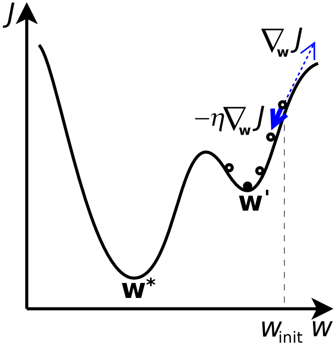

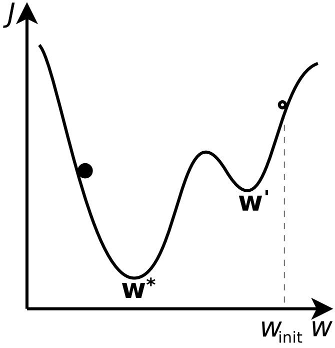

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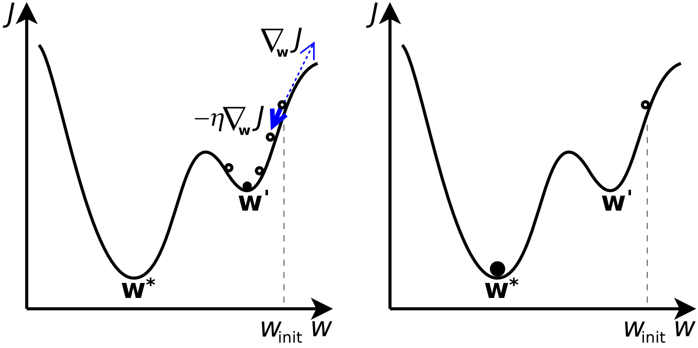

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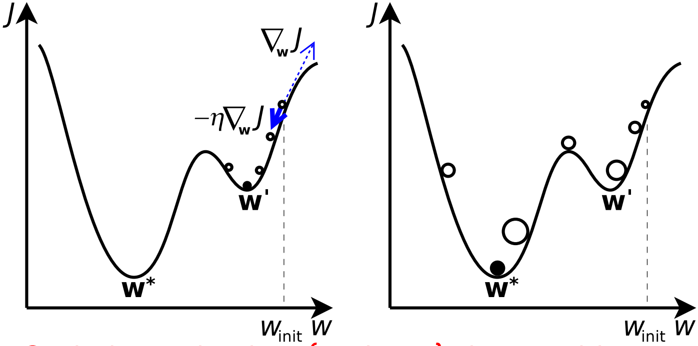


Optimizer selection: (perhaps) via searching..

Optimizers

Or solvers in Scikit-learn..

sklearn.neural_network.MLPRegressor

class `sklearn.neural_network.`**`MLPRegressor`**(*hidden_layer_sizes=(100,), activation='relu', *, solver='adam', alpha=0.0001, batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000*) [source]

Multi-layer Perceptron regressor.

This model optimizes the squared-loss using LBFGS or stochastic gradient descent.

New in version 0.18.

Parameters:

hidden_layer_sizes : *tuple, length = n_layers - 2, default=(100,)*

The ith element represents the number of neurons in the ith hidden layer.

solver : *{'lbfgs', 'sgd', 'adam'}, default='adam'*

The solver for weight optimization.

- 'lbfgs' is an optimizer in the family of quasi-Newton methods.
- 'sgd' refers to stochastic gradient descent.
- 'adam' refers to a stochastic gradient-based optimizer proposed by Kingma, Diederik, and Jimmy Ba

Note: The default solver 'adam' works pretty well on relatively large datasets (with thousands of training samples or more) in terms of both training time and validation score. For small datasets, however, 'lbfgs' can converge faster and perform better.

activation : *{'identity', 'logistic', 'tanh', 'relu'}, default='relu'*

Activation function for the hidden layer.

Optimizers

Or optimizers in Keras..

Available optimizers

- SGD
- RMSprop
- Adam
- Adadelta
- Adagrad
- Adamax
- Nadam
- Ftrl

K + TensorFlow

K Keras

Search Keras documentation...

- About Keras
- Getting started
- Developer guides
- Keras API reference
  - Models API
  - Layers API
  - Callbacks API
  - Data preprocessing
  - Optimizers
  - Metrics
  - Losses
  - Built-in small datasets
  - Keras Applications
  - Utilities
- Code examples
- Why choose Keras?

» Keras API reference / Optimizers

Optimizers

Usage with `compile()` & `fit()`

An optimizer is one of the two arguments required for compiling a Keras model:

```
from tensorflow import keras
from tensorflow.keras import layers

model = keras.Sequential()
model.add(layers.Dense(64, kernel_initializer='uniform', input_shape=(10,)))
model.add(layers.Activation('softmax'))

opt = keras.optimizers.Adam(learning_rate=0.01)
model.compile(loss='categorical_crossentropy', optimizer=opt)
```

You can either instantiate an optimizer before passing it to `model.compile()` , as in the above example, or you can pass it by its string identifier. In the latter case, the default parameters for the optimizer will be used.

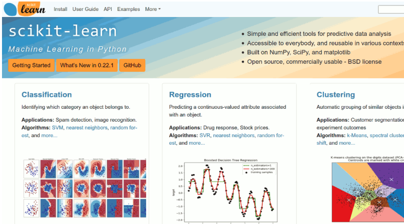
```
# pass optimizer by name: default parameters will be used
model.compile(loss='categorical_crossentropy', optimizer='adam')
```

ML Models (or ML algorithms)

Models encountered so far

Some classifiers and regressors..

```
sklearn.neighbors.KNeighborsRegressor
sklearn.linear_model.LinearRegression
sklearn.linear_model.SGDClassifier
sklearn.linear_model.SGDRegressor
```



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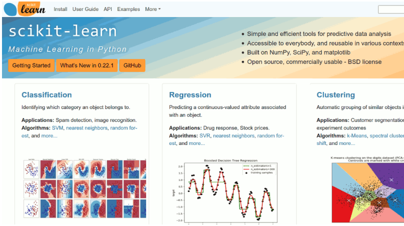

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Perhaps..

- `sklearn.naive_bayes.GaussianNB`
- `sklearn.naive_bayes.MultinomialNB`
- `sklearn.svm.SVC`
- `sklearn.svm.SVR`

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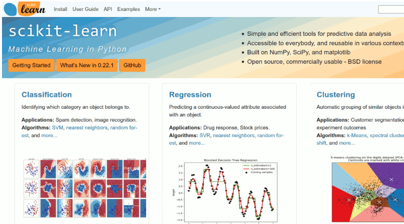

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and to some degree..

`sklearn.linear_model.LogisticRegression`
`sklearn.linear_model.Perceptron`
`sklearn.neural_network.MLPClassifier`
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`keras.Sequential`

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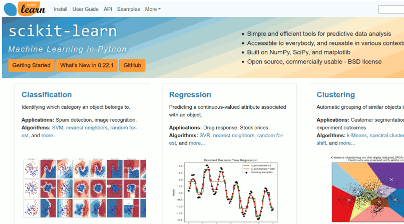

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keras.Sequential
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Or even more exotic models like..

- superviced ensemble: AdaBoost, Bagging, DecisionTree, RandomForest,..
- semi-supervised: ??
- unsupervised: K-means, manifolds, restricted Boltzmann machines,..
- clustering: K-means

ML Algorithm + Model Selection via Searching

What ML algorithm to choose?

- manual:

  algorithm characteristics, $\mathcal{O}$ complexity, etc.
  browsing through Scikit-learn documentation,
  ...and also based on data assumptions.

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```
models = {
  SVC(gamma="scale"),
  SGDClassifier(tol=1e-3, eta0=0.1),
  GaussianNB()
}

for i in models:
    i.fit(X_train, y_train)
    y_pred_test = i.predict(X_test)
    p = precision_score(y_test, y_pred_test, average='micro')
    print(f'{type(i).__name__:13s}: precision={p:0.2f}')
```

NOTE: Python set = {`a, b`}
Python dictionary= {`a:x, b:y`}

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prints..

```
GaussianNB:    p=1.00
SGDClassifier: p=0.93
SVC:           p=0.98
```

NOTE: Python set = `{a, b}`
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Model Selection via Grid Search

The hyperparamter-set for SGD linear regressor

```
class sklearn.linear_model.SGDRegressor(
  loss    ='squared_loss', penalty     ='l2',
  alpha   =0.0001,         l1_ratio    =0.15,
  tol     =None,           shuffle     =True,
  verbose =0,              epsilon     =0.1,
  eta0    =0.01,           power_t     =0.25,
  n_iter_no_change=5,      warm_start  =False,
  fit_intercept   =True,   max_iter    =None,
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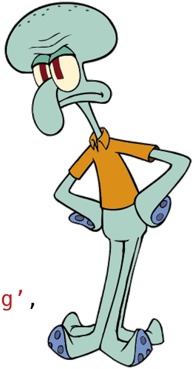

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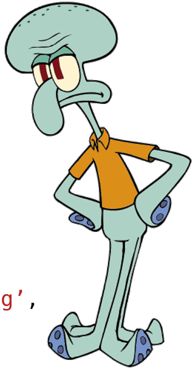

Search best hyperparameters in a (smaller) set, say

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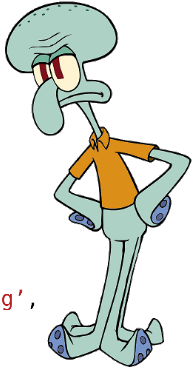

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```

Search best hyperparameters in a (smaller) set, say

```
model = SGDClassifier()
tuning_parameters = {
  'alpha': [ 0.001, 0.01, 0.1],
  'max_iter': [1, 10, 100, 100],
  'learning_rate':('constant','optimal','invscaling','adaptive')
}
..
grid_tuned = GridSearchCV(model, tuning_parameters, ..
```

Model Selection via Grid Search

How to select 'best' set of hyperparameter—using bute force?

Gridsearch seen in 3D for the two hyperspace dimensions:

- `alpha` $\in [1, 2, 3, ..]$
- `max_iter` $\in [1, 2, 3, ..]$

(NOTE: linear range for this plot only, should be 1, 10, 100 or similar.)

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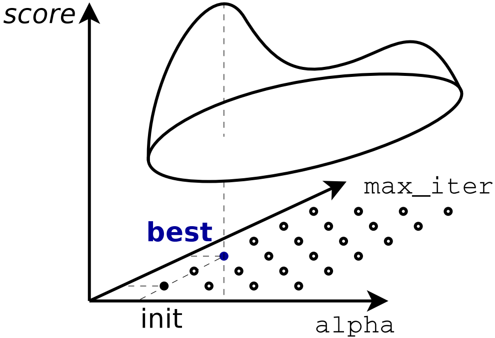

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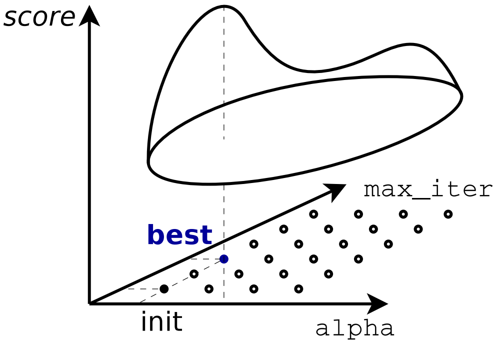

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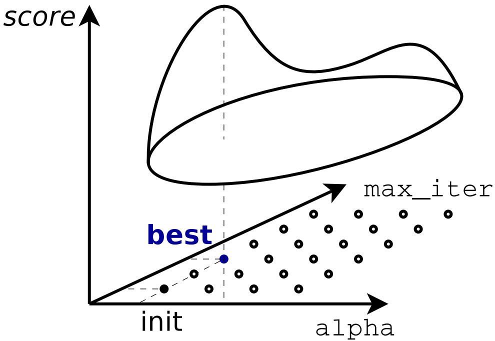

- why `score` and not J on $z-$axis?
- and what if there are many hyperparameters and many combinations? $\rightarrow$ Zzzzzzz!

Model Selection via Randomized Search

How to select 'best' set of hyperparameters—faster than brute force?

Replace `GridSearchCV()` with

```
RandomizedSearchCV(n_iter=100,..)
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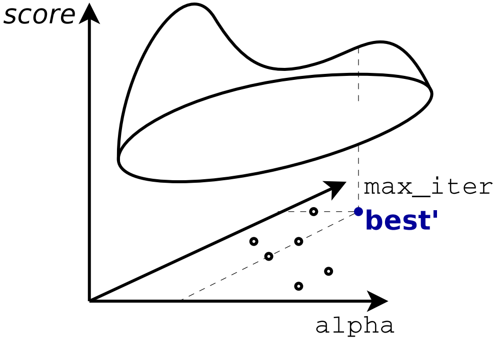

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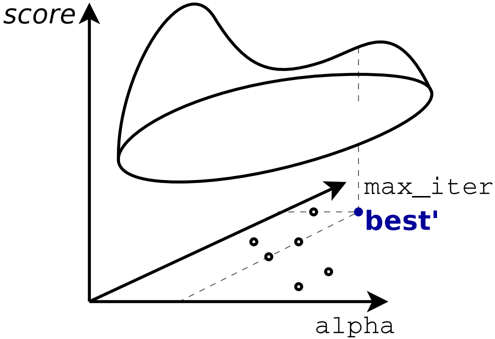

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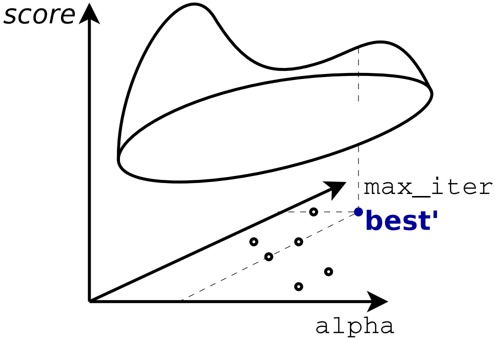
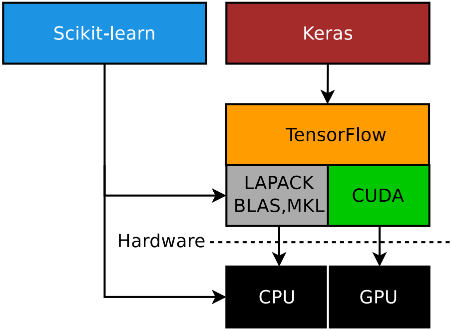


- faster, but will not yield the (sub) optimal score maximum,
- ...but does it matter in a huge hyperparameter search-space?

Extra Slides..

Keras and Tensorflow

Using the Keras API instead of Scikit-learn or TensorFlow



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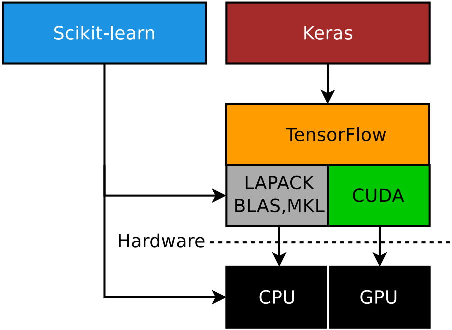

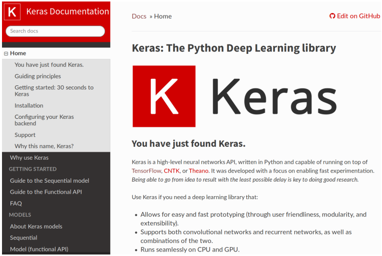

NOTE:

- documentation: `https://keras.io/`

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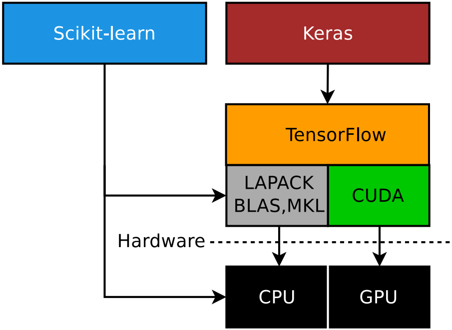
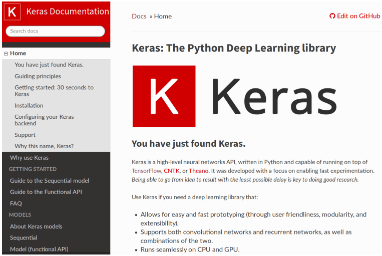
Using the Keras API instead of Scikit-learn or TensorFlow



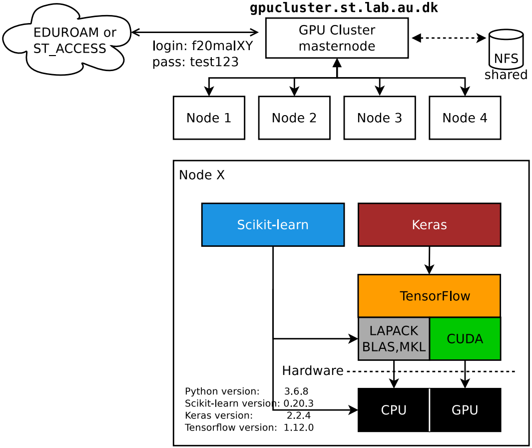


NOTE:

- documentation: `https://keras.io/`
- keras provides a `fit-predict`-interface,
- many similiarities to Scikit-learn,
- but also many differences!

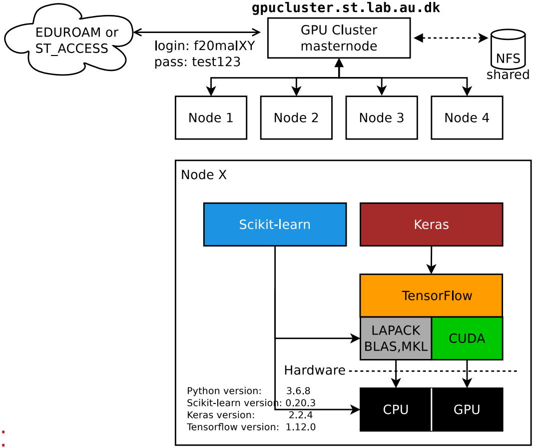
High-Performace-Computing (HPC)

Running on the ASE GPU cluster, your group login=e20malXY



High-Performace-Computing (HPC)

Running on the ASE GPU cluster, your group login=e20malXY



NOTE:

manuel GPU hukommelses Garbage Collection...

For `keras` GPU kald:

```
StartupSequence_EnableGPU(gpu_mem_fraction=0.1, gpus=1)
```

NOTE2: script found in `/home/shared/00_init.py` that runs for all users!