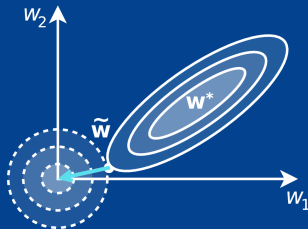




## Lesson 09: Regularization, Optimization and Searching

CARSTEN EIE FRIGAARD

AUTUMN 2024



"A computer program is said to learn from experience  $E$  with respect to some class of tasks  $T$  and performance measure  $P$ , if its performance at tasks in  $T$ , as measured by  $P$ , improves with experience  $E$ ." — Mitchell (1997).

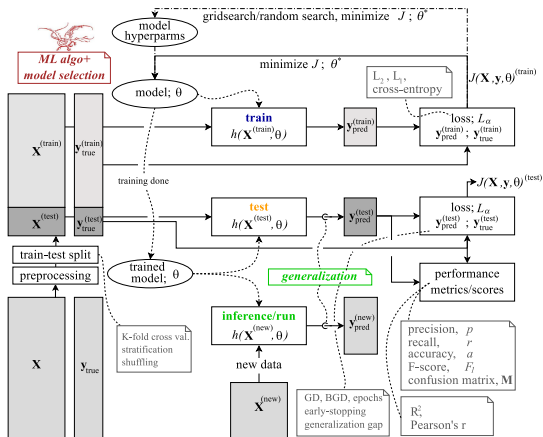
# Agenda

- ▶ **Resumé: ML Algorithm and Model Selection:**  
k-fold Cross-Validation revisited,
- ▶ **Regularization:**  
Regulizers,  
Exercise: ~~L09/regulizers.ipynb~~ (F24)  
(no exercise, E24)
- ▶ **Optimizers:**  
(no exercise).
- ▶ **Searching:**  
Gridsearch,  
Randomsearch,  
Exercise: ~~L09/gridsearch.ipynb~~

# ML Algorithm Selection and Model Selection

## Manually Choosing an Algorithm and Tuning a Model..

- ▶ algorithm selection.
- ▶ model selection,
- ▶ model evaluation,
- ▶ **re-iteration and re-selection!**



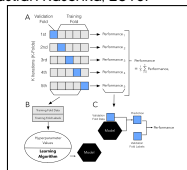
### Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning

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  $k$ -tree  $N$ -fold 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.



# ML Algorithm Selection and Model Selection

Manually Choosing an Algorithm and Tuning a Model..

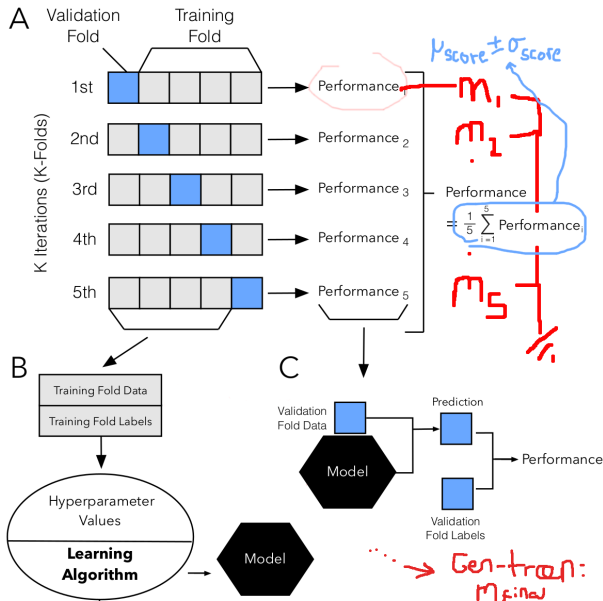
- ▶ algorithm selection:
  - ▶ choose an algo that '*fits*' the problem, ...perhaps via searching??
- ▶ model selection:
  - ▶ looking for 'optimal' model capacity,
  - ▶ tuning model **hyperparameters**..
    - ▶ model weights **regularizers**..(for NN's)
    - ▶ gradient descent **optimizers**..(for NN's)
- ▶ model evaluation:
  - ▶ 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)..
- ▶ **re-iteration and re-selection!**



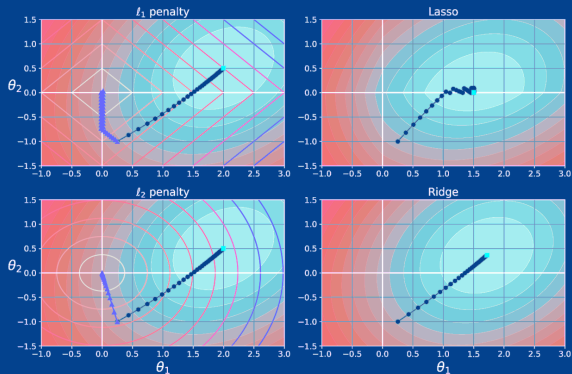
**NOTE:** Model selection: ~ selection the best capacity/hyperparameter for a given model—NOT choosing the ML algo/model itself!

# Model Evaluation

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



# REGULARIZATION



# Regularization

## Adding a Penalty to the Cost Function

For a linear regressor, our cost function was

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

But now enters a **penalty factor**,  $\Omega$ , that scaled with  $\alpha$  adds extra cost to  $J$ ,

$$\tilde{J}(\mathbf{X}, \mathbf{y}; \mathbf{w}) = ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \alpha\Omega(\mathbf{w})$$

so this becomes **a-tug-of-war** between the two terms in  $\tilde{J}$ .

The effect of the added penalty is to:

- ▶ put a **constraint** on the norm of the weights,  $\mathbf{w}$ , disallowing 'em to grow wildly,
- ▶ 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

$$\Omega(\mathbf{w}) = \|\mathbf{w}\|_2^2 = \mathbf{w}^\top \mathbf{w}$$

$$\tilde{J}_{\text{ridge}}(\mathbf{X}, \mathbf{y}; \mathbf{w}) = J(\mathbf{X}, \mathbf{y}; \mathbf{w}) + \alpha \mathbf{w}^\top \mathbf{w}$$

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

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

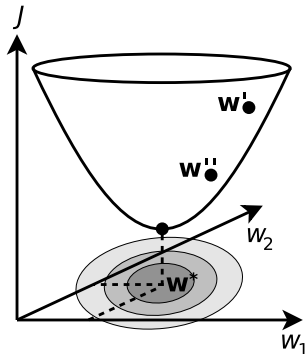
**NOTE:** ..and give-or-take some additional  $1/2$  or  $1/n$  constant, that we do not care about.



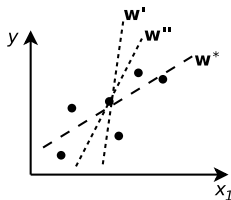
# $\mathcal{L}_2$ Regularization

## Ridge Penalization

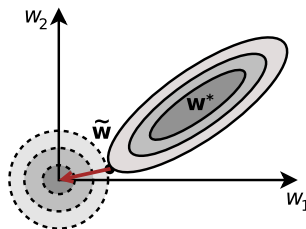
A graphical view for a linear regressor



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



1D featurespace



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

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

$$\Omega(\mathbf{w}) = \|\mathbf{w}\|_1$$

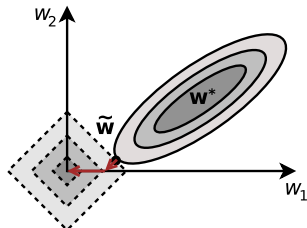
$$\tilde{J}_{\text{lasso}}(\mathbf{X}, \mathbf{y}; \mathbf{w}) = J(\mathbf{X}, \mathbf{y}; \mathbf{w}) + \alpha \|\mathbf{w}\|_1$$

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 sparse model,
- ▶ i.e few nonzero  $w$ 's.



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

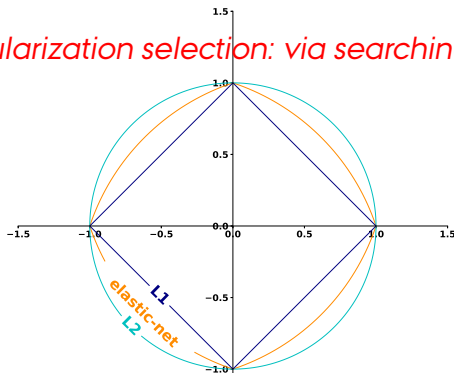
## Elastic-net Penalization

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

$$\Omega(\mathbf{w}) = \beta \|\mathbf{w}\|_1 + (1 - \beta) \|\mathbf{w}\|_2^2$$

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

*Regularization selection: via searching..*



# HOML Fig 4-19 Explained

You can get a sense of why this is the case by looking at Figure 4-19: on the top-left plot, the background contours (ellipses) represent an unregularized MSE cost function ( $\alpha = 0$ ), and the white circles show the Batch Gradient Descent path with that cost function. The foreground contours (diamonds) represent the  $\ell_1$  penalty, and the triangles show the BGD path for this penalty only ( $\alpha \rightarrow \infty$ ). Notice how the path first reaches  $\theta_1 = 0$ , then rolls down a gutter until it reaches  $\theta_2 = 0$ . On the top-right plot, the contours represent the same cost function plus an  $\ell_1$  penalty with  $\alpha = 0.5$ . The global minimum is on the  $\theta_2 = 0$  axis. BGD first reaches  $\theta_2 = 0$ , then rolls down the gutter until it reaches the global minimum. The two bottom plots show the same thing but uses an  $\ell_2$  penalty instead. The regularized minimum is closer to  $\theta = \mathbf{0}$  than the unregularized minimum, but the weights do not get fully eliminated.

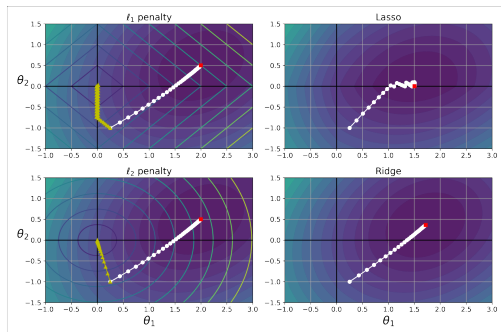


Figure 4-19. Lasso versus Ridge regularization



On the Lasso cost function, the BGD path tends to bounce across the gutter toward the end. This is because the slope changes abruptly at  $\theta_2 = 0$ . You need to gradually reduce the learning rate in order to actually converge to the global minimum.

# HOML fig 4-19 Explained

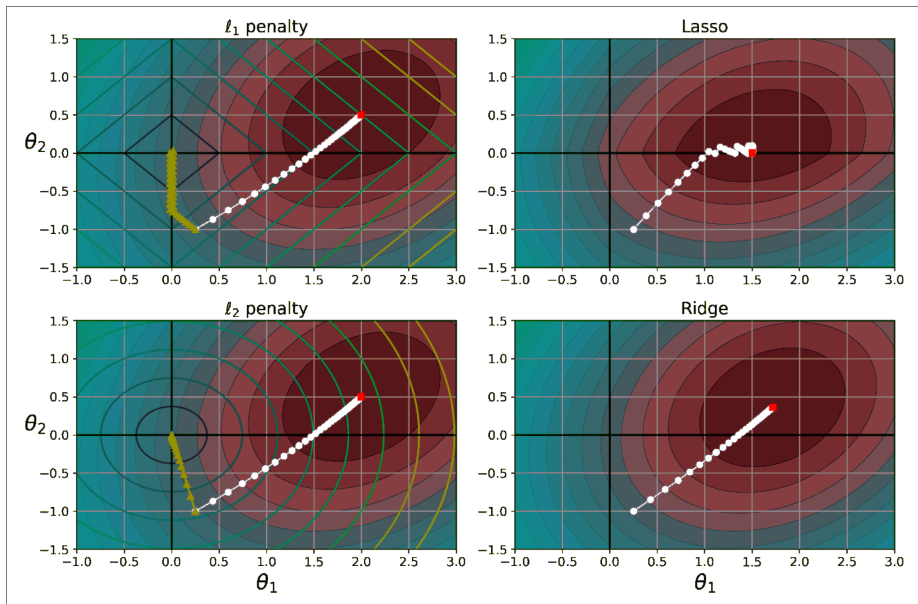
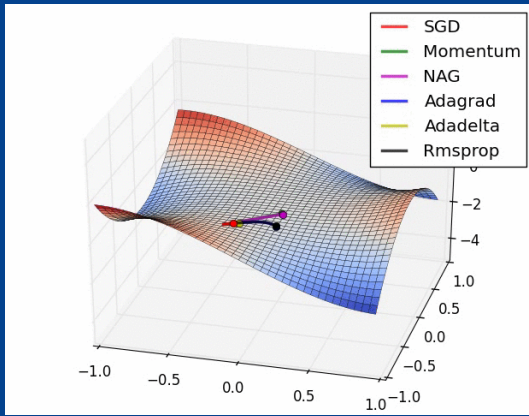


Figure 4-19. Lasso versus Ridge regularization

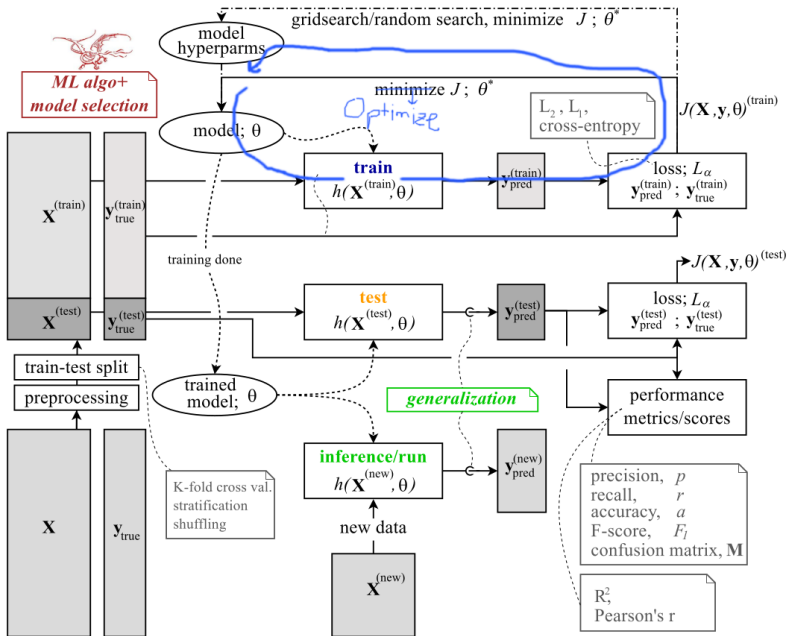
# OPTIMIZERS

---



CLICK ME (mp4)!

# Optimizers



# Optimizers

## Momentum Optimization

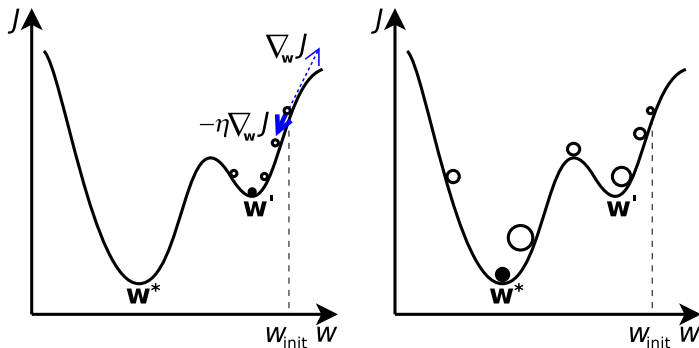
Normal GD algo

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

but now with added (physical) momentum

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

$$\mathbf{w} \leftarrow \mathbf{w} + \mathbf{m}$$



*Optimizer selection: (perhaps) via searching..*



### `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 *i*th element represents the number of neurons in the *i*th 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..



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?

Search Keras documentation...

» 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')
```

## Available optimizers

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



### Optimizers

- ▷ Usage with `compile()` & `fit()`
- ▷ Usage in a custom training loop
- ▷ Learning rate decay scheduling
- ▷ Available optimizers
- ▷ Core Optimizer API
  - apply\_gradients method
  - weights property
  - get\_weights method
  - set\_weights method

# Optimizers Demo

L09/Extra/intro\_mlp\_revisited.ipynb

jupyter intro\_mlp\_revisited Last Checkpoint: 1 mandags kl. 09:47 (autosaved)



Logout

File Edit View Insert Cell Kernel Widgets Help

Connecting to kernel

Trusted

Python 3

Run Markdown

## ITMAL Demo

MLP demo of solvers and a 1-neuron MLP for the OECD data from intro.

In [3]:

```
1 %matplotlib inline
2
3 import numpy as np
4 import matplotlib
5 import matplotlib.pyplot as plt
6
7 def LoadDataFromL01():
8     import pickle
9     filename = "../L04/Data/itmal_l01_data.pkl"
10    with open(f"{filename}", "rb") as f:
11        (X, y) = pickle.load(f)
12        return X, y
13
14 X, y = LoadDataFromL01()
15
16 print(f"X.shape={X.shape}, y.shape={y.shape}")
17
18 assert X.shape[0] == y.shape[0]
19 assert X.ndim == 2
20 assert y.ndim == 1 # did a y.ravel() before saving to pickle file
21 assert X.shape[0] == 29
22
23 # re-create plot data (not stored in the Pickle file)
24 m = np.linspace(0, 60000, 1000)
25 M = np.empty([m.shape[0], 1])
26 M[:, 0] = m
27
28 print("OK")
```

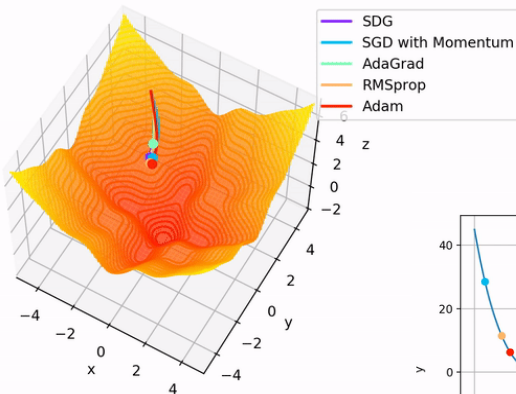
X.shape=(29, 1), y.shape=(29,)

OK

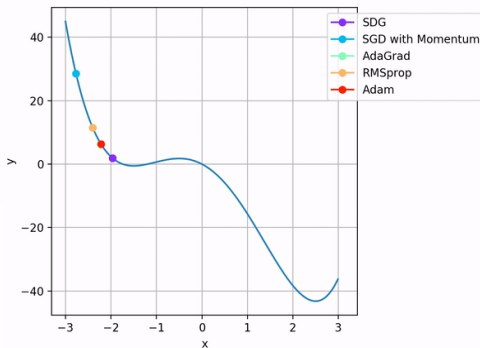
# Optimizers

CLICK US (mp4s)!

Optimizer Comparison



Optimizer Comparison



Sources: Imgur by Alec Radford and  
<https://towardsdatascience.com/complete-guide-to-adam-optimization-1e5f29532c3d>

# SEARCHING

---

ML Algorithm +  
Model Selection via Searching



# 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
```

### Perhaps..

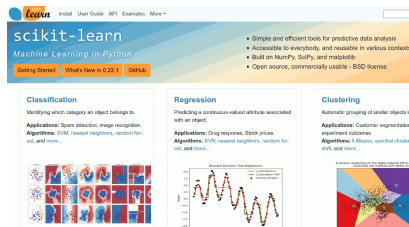
```
sklearn.naive_bayes.GaussianNB  
sklearn.naive_bayes.MultinomialNB  
sklearn.svm.SVC  
sklearn.svm.SVR
```

### and to some degree..

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

### Or even more exotic models like..

- ▶ supervised 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 at what Model Capacity?

► manual:

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

► semi-automatic:

brute-force model search, and fun with python!

```
1 models = {  
2     SVC(gamma="scale"),  
3     SGDClassifier(tol=1e-3, eta0=0.1),  
4     GaussianNB()  
5 }  
6  
7 for i in models:  
8     i.fit(X_train, y_train)  
9     y_pred_test = i.predict(X_test)  
10    p = precision_score(y_test, y_pred_test, average='micro')  
11    print(f'{type(i).__name__:13s}: precision={p:0.2f}')
```

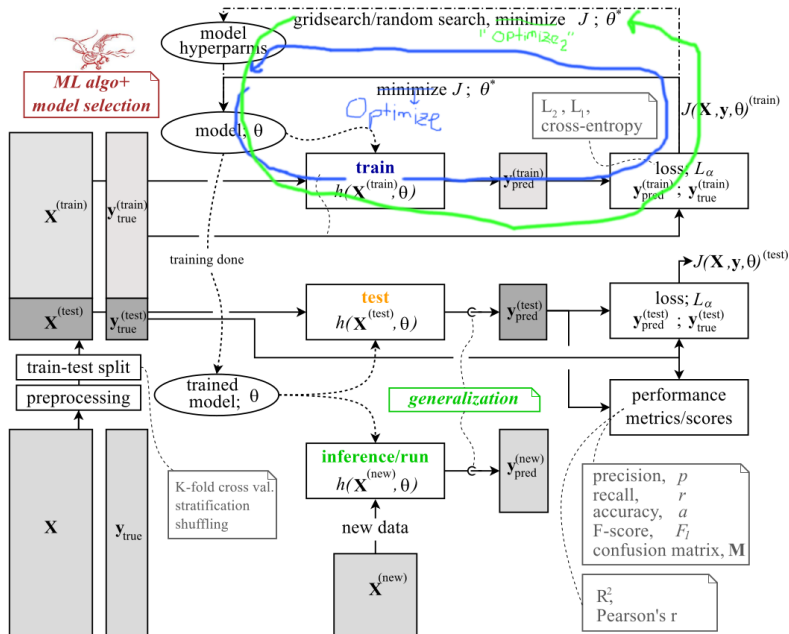
prints..

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

NOTE: Python set = {a, b}

Python dictionary= {a:x, b:y}

# Model Selection via Grid Search





# Model Selection via Grid Search

The hyperparameter-set for SGD linear regressor

```
1 class sklearn.linear_model.SGDRegressor(  
2     loss      = 'squared_loss', penalty      = 'l2',  
3     alpha     = 0.0001,               l1_ratio   = 0.15,  
4     tol       = None,                 shuffle    = True,  
5     verbose   = 0,                   epsilon    = 0.1,  
6     eta0      = 0.01,                power_t    = 0.25,  
7     n_iter_no_change=5,               warm_start  = False,  
8     fit_intercept = True,             max_iter    = None,  
9     average     = False,             n_iter      = None,  
10    random_state  = None,             learning_rate='invscaling',  
11    early_stopping = False,           validation_fraction=0.1  
12 )
```



Search best hyperparameters in a (smaller) set, say

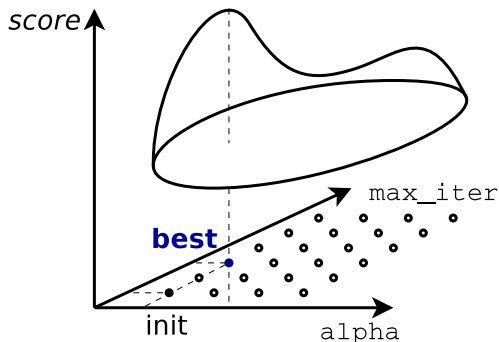
```
1 model = SGDRegressor()  
2 tuning_parameters = {  
3     'alpha': [ 0.001, 0.01, 0.1],  
4     'max_iter': [1, 10, 100, 1000],  
5     'learning_rate': ('constant', 'optimal', 'invscaling', 'adaptive')  
6 }  
7 ..  
8 grid_tuned = GridSearchCV(model, tuning_parameters, ..
```

# Model Selection via Grid Search

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

Gridsearch seen in 3D for the two hyperspace dimensions:

- ▶  $\alpha \in [1, 2, 3, \dots]$  (NOTE: linear range for this plot only,
- ▶  $\text{max\_iter} \in [1, 2, 3, \dots]$  should be 1, 10, 100 or similar.)



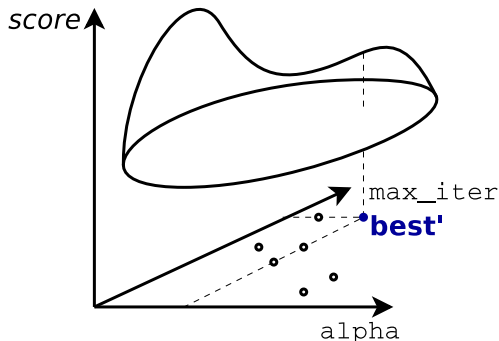
- ▶ why score and not  $J$  on  $z$ -axis?
- ▶ and what if there are many hyperparameters and many combinations?  $\rightarrow$  Zzzzzzz!

# Model Selection via Randomized Search

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

Replace `GridSearchCV()` with

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




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

# Exercise: L09/gridsearch.ipynb

## Qd MNIST Search Quest II: Husk at publicer på Brightspace

<i>L08:</i> Regular: × +

https://blackboard.au.dk/webapps/blackboard/content/listContentEditable.jsp?content\_id=\_2931033\_1&course\_id=\_145075 120% ...



### Qd MNIST Search Quest II

Publicer (helt nederst i denne item) løbende dit bedste resultat fra opgaven

gridsearch.ipynb (Qd)

Indtast din model constructor string og score og en kommentar vdr. dit model ala

```
Grp09: best: dat=mnist, score=0.90780, model=SGDClassifier(alpha=1.0,eta0=0.0001,learning_rate='invscaling')
```

```
Grp09: CTOR for best model: SGDClassifier(alpha=1.0, average=False, class_weight=None, early_stopping=False, epsilon=0.1, eta0=0.0001, fit_intercept=True, l1_ratio=0.15, learning_rate='invscaling', loss='hinge', max_iter=1000, n_iter_no_change=5, n_jobs=None, penalty='l2', power_t=0.5, random_state=None, shuffle=True, tol=0.001, validation_fraction=0.1, verbose=0, warm_start=False)
```

NB: brug af **neurale netværks** modeller (Perceptrons, MLP's, Keras etc.) samt **KNeighborsClassifier** ikke tilladt i denne quest!

**Highscore fra sidste semester = 0.97369**

```
model=KNeighborsClassifier(algorithm='ball_tree', n_neighbors=3, p=4,weights='distance')
```

### ITMAL Search Quest

Send message...

VERSION: 0.0.0

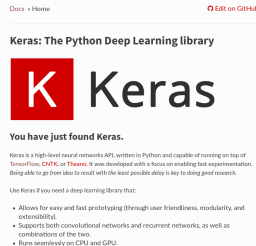
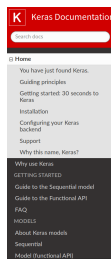
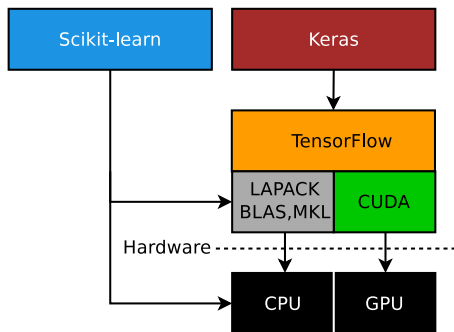
8/32

Extra Slides..

# Keras and Tensorflow



Using the Keras API instead of Scikit-learn or TensorFlow



NOTE:

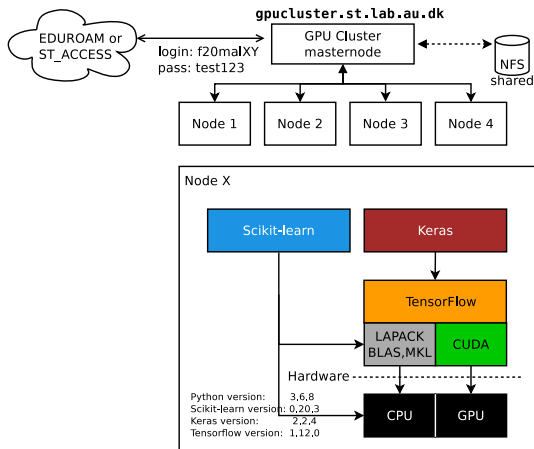
- ▶ documentation: <https://keras.io/>
- ▶ keras provides a `fit-predict`-interface,
- ▶ many similarities to Scikit-learn,
- ▶ but also many differences!

# High-Performance-Computing (HPC)

Running on the ASE GPU Cluster:

login=swmal09f24 (for SWMAL group 9)

password=swmal09f24\_123



# GPU Cluster: Updated Architecture

