AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

MACHINE LEARNING

LESSON 7: Optimization and Searching

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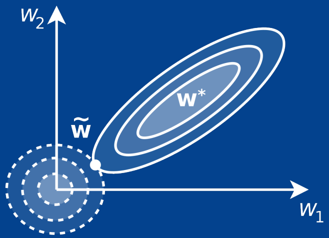
SPRING 2019



L07: Optimization and Searching

Agenda

- BB | Hand-ins Deadlines | Selected J1 hand-ins
- GPU Cluster via EDUROAM or VPN/au-access
  (but loss of port 22)
- Regularization and Optimization
  Preprocessing of data (no-exe),
  Optimizers (no-exe),
  Regulizers,
  Exercise: `L07/regulizers.ipynb`
- Searching
  Model selection and model searching (no-exe),
  Gridsearch,
  Randomsearch,
  Exercise: `L07/gridsearch.ipynb`

Preprocessing of Data

Scaling, Standardization, Normalization...

Why the need for preprocessing?

> *Standardization of datasets is a* **common requirement for many machine learning estimators** *[..]; they might* **behave badly** *if the individual features do not more or less look like standard normally distributed data. [..]*
>
> [`https://scikit-learn.org/stable/modules/preprocessing.html`]

Standardization of a feature vector $\mathbf{x}$, giving $\mathbf{x}'$ mean zero, and standard deviation one

$$\mathbf{x}' = \frac{\mathbf{x} - \mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}}$$

What kind of estimators needs standardization?

$\rightarrow$ **Neural networks (NNs) in particular!**

Regularization and optimization:

$\rightarrow$ WARM-UP for the comming use of NNs!

Preprocessing of Data

Scaling, Standardization, Normalization...

Common preprocessing methods

- standardization, aka mean/std scaling, $\frac{x-\mu}{\sigma}$
  `sklearn.preprocessing.StandardScaler`
- min/max, or abs scaling, say $x \in [0; 1]$
  `sklearn.preprocessing.MinMaxScaler`
  `sklearn.preprocessing.MaxAbsScaler`
- normalization, giving unit norm
  `sklearn.preprocessing.normalize`

Potential problems:

- outliers,
- NaNs (Not-a-Number)

Preprocessing of Data

Scaling, Standardization, Normalization in a Pipeline

Use preprocessing as first state in a fit-predict **pipeline**

```
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import make_pipeline
from sklearn.naive_bayes import GaussianNB

mypipeline = make_pipeline(
    StandardScaler(),
    GaussianNB()
)

..
mypipeline.fit(X_train, y_train)
..
mypipeline.predict(X_test)
```

[[GITMAL],L07/Extra/standardization_demo.ipynb]

Remember: scale train and test equally!

Regularization

Adding a Penalty to the Cost Function

For a linear regressor, our cost function was

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

But now enters a **penalty factor**, Ω, adding extra cost to J, and scaled with α

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

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

The effect of the added penalty is to:

- put a **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 Penalisation

Aka Weight Decay, aka Tikhonov regularization

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

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

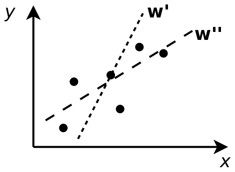
$$\mathcal{L}_2^2 : ||\mathbf{x}||_2^2 = \mathbf{x}^\top \mathbf{x}$$

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

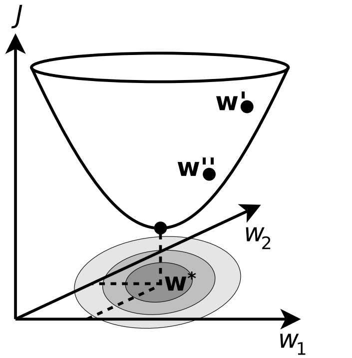
$\mathcal{L}_2$ Regularization

Ridge Penalization

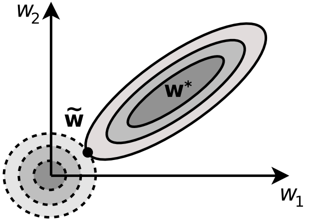
A graphical view for a linear regressor



2D $y - x$ space,
here only 1D shown.



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



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

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

with the Manhattan norm

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

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

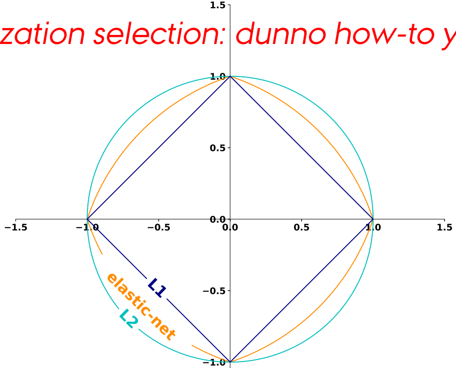
Elastic-net Penalisation

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

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

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

Regularization selection: dunno how-to yet!??



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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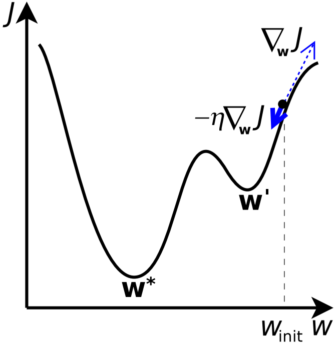

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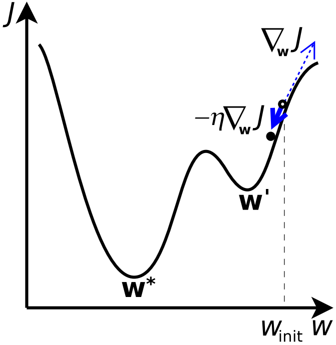

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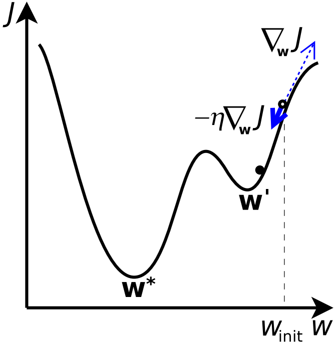

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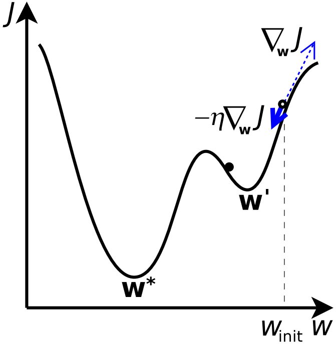

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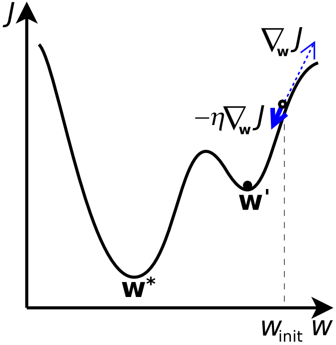

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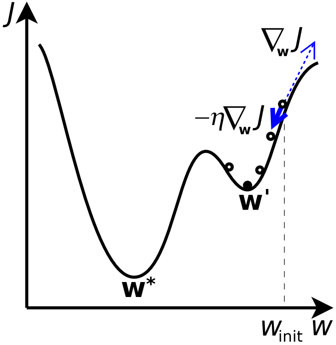

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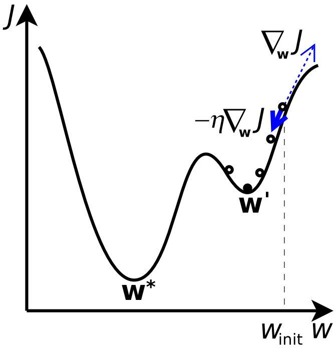

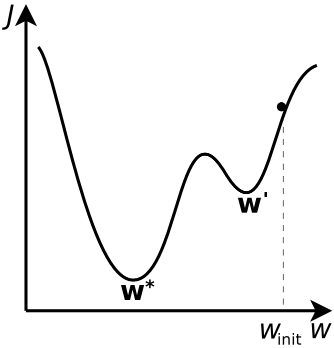

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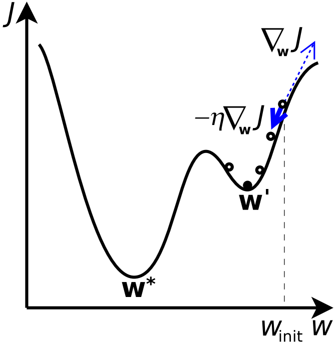

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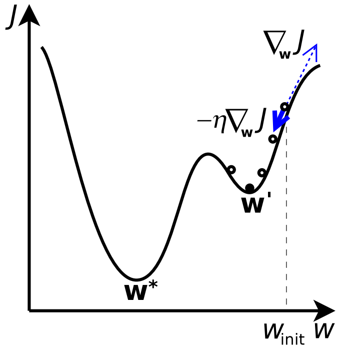

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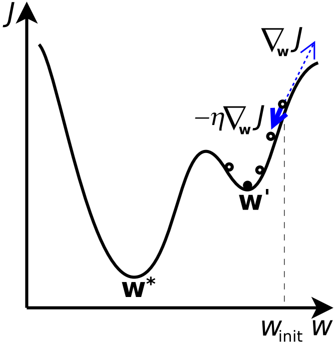

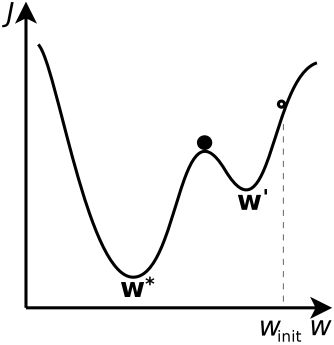

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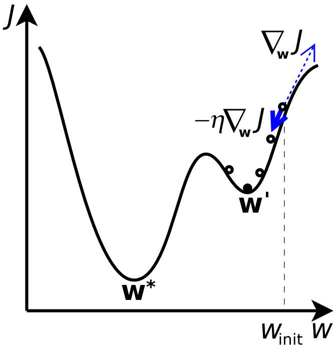

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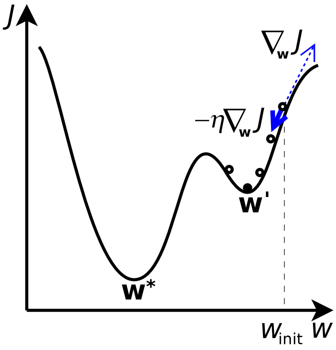

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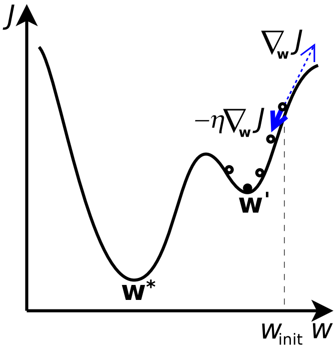

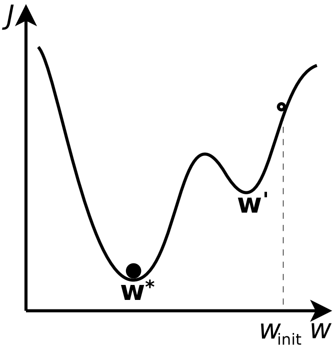

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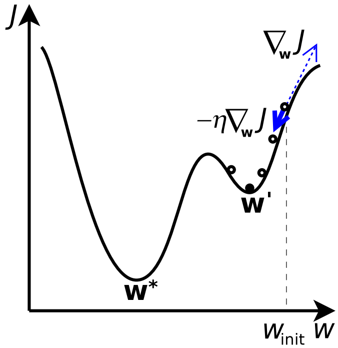


ML Models

Models Encountered so far

Some classifiers and regressors..

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

Perhaps...

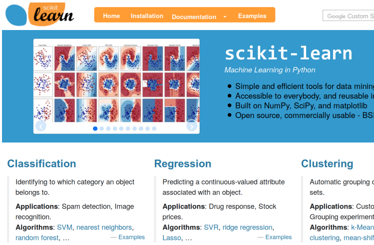
```
sklearn.naive_bayes.GaussianNB
sklearn.naive_bayes.MultinomialNB
```

Not really or not in depth

```
sklearn.linear_model.Perceptron
sklearn.linear_model.LogisticRegression
sklearn.svm.SVC
sklearn.svm.SVR
sklearn.neural_network.MLPClassifier
sklearn.neural_network.MLPRegressor
```

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 Model Selection and Searching

What ML model to choose?

Model selection

- manual:
  model characteristics, $\mathcal{O}$ complexity, etc.
  browsing through Scikit-learn documentation,
  ...and also based on data assumptions.
- semi-automatic:
  model search, and fun with python!

```
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}')
```

prints..

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

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

Model Hyperparameters 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,
  average         =False,  n_iter       =None
  random_state    =None,   learning_rate='invscaling',
  early_stopping =False,   validation_fraction=0.1
)
```

Search best hyperparameters in a (smaller) set, say

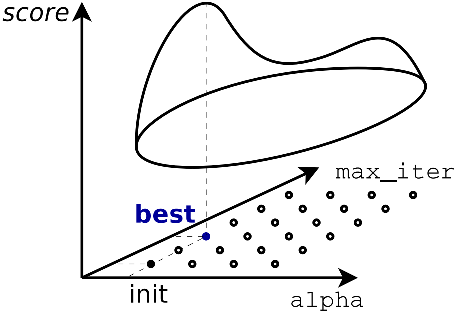
```
model = SGDClassifier()
tuning_parameters = {
  'alpha': [ 0.001, 0.01, 0.1],
  'max_iter': [1, 10, 100, 100],
  'learning_rate':('constant','optimal','invscaling','adaptive')
}
..
grid_tuned = GridSearchCV(model, tuning_parameters, ..
```

Model Hyperparameters Grid Searching

How to set hyperparameters optimally?

Gridsearch seen in 3D for the two hyperspace dimensions:

- `alpha` $\in [1, 2, 3..]$ (NOTE: linear range for this plot only!),
- `learnig_rate` $\in [1, 2, 3..]$



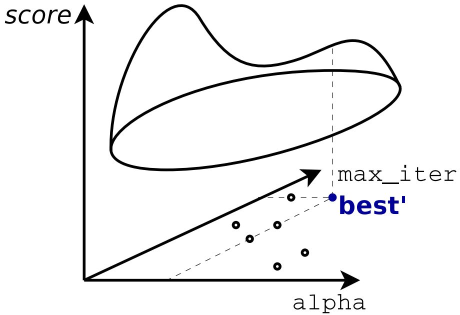
But, what if there are many hyperparameters and many combinations? $\rightarrow$ Zzzzzzz!

Model Hyperparameters Random Searching

How to set hyperparameters faster but less optimally?

Replace `GridSearchCV()` with

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



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