Machine learning and physical modelling-3

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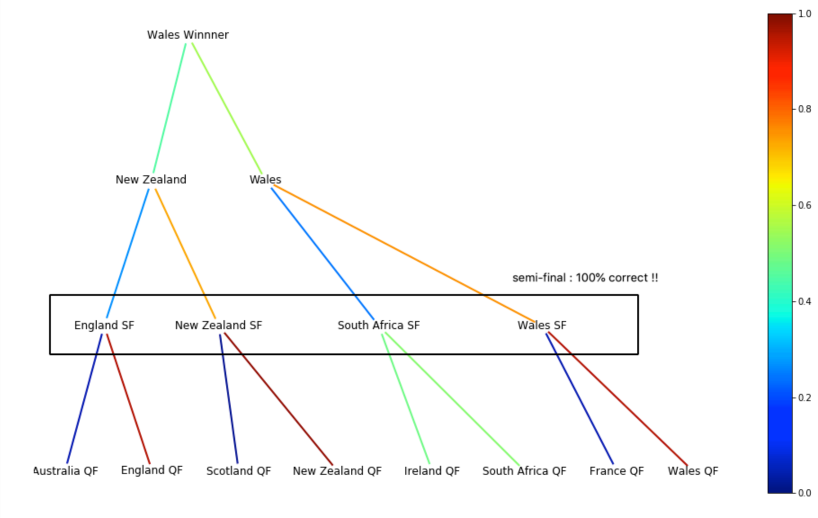
NERSC

https://github.com/brajard/MAT330

Have a look at the Rugby world cup?



But if we look at the easiest predictor....

FULL RANKINGS

POSITION		TEAMS	POINTS
1	(1)	NEW ZEALAND	92.47
2	(3)	ENGLAND	89.74
3	(2)	WALES	89.37
4	(5)	SOUTH AFRICA	88.55

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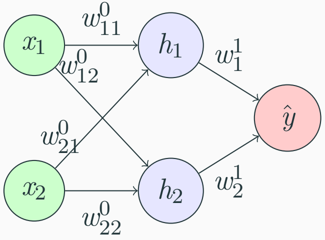
Gradient backpropagation

Training a neural-net: gradient backpropagation



Objective

Determination of the best set of weights $\mathbf{w}$ to minimize the Loss function $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2$.

Calculation of $\partial L / \partial w$

1. Given a couple (x, y)

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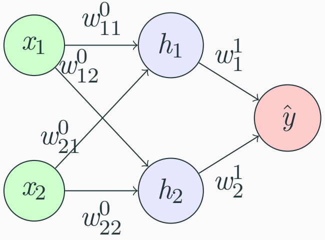

1. Given a couple (x, y)
2. Forward computation:
   $h_j = f_0(\sum_{i=1}^{2} w^0_{ij}.x_i)$
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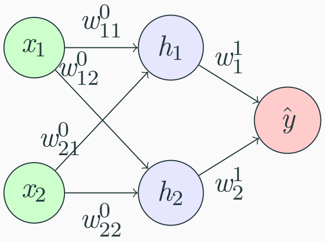

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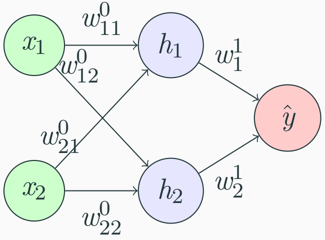

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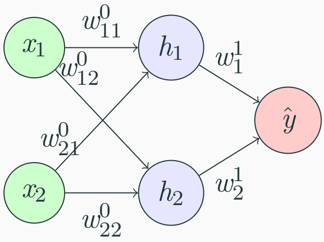

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   - Layer 1
     $\partial L/\partial w^1_j = \boxed{\partial L/\partial \hat{y}}.\partial f_1/\partial w^1_j$
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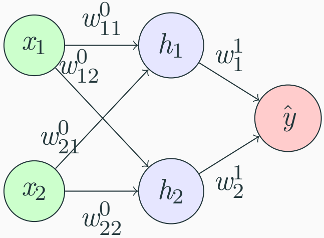

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   - Layer 0
     $\partial L/\partial w^0_{ij} = \boxed{\partial L/\partial h_j}.\partial f_1/\partial w^0_{ij}$

Optimizing a machine learning (gradient method)

Optimizing the loss

Several loss function (depending on the problem) can be defined.

For example, Mean Square Error:

Method

Find a minimum of L by adjustig the parameters (weights) $\mathbf{w}$ given the gradient of the loss with respect to the weights $\nabla_{\mathbf{w}} L$.

Batch Vs Stochastic training

Dataset: (X, Y) with N samples denoted $(\mathbf{x_i}, y_i)$

Batch gradient:

Require: Learning rate(s): ν_k
Require: Initial weights: $\mathbf{w}$
  $k \leftarrow 1$
  while stopping criterion not met **do**
    Compute gradient:
  $\mathbf{g} \leftarrow \frac{1}{N}\sum_i^N \nabla_{\mathbf{w}} L(f(\mathbf{x}_i, y_i))$
    Update weights: $\mathbf{w} \leftarrow \mathbf{w} - \nu_k \mathbf{g}$
    $k \leftarrow k+1$
  end while

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1 Update / N forwards

Stochastic gradient:

Require: Learning rate(s): ν_k
Require: Initial weights: $\mathbf{w}$
$k \leftarrow 1$
while stopping criterion not met **do**
Sample an example $(\mathbf{x}, y)$ from (X, Y)
Compute gradient: $\mathbf{g} \leftarrow \nabla_{\mathbf{w}} L(f(\mathbf{x}, y))$
Update weights: $\mathbf{w} \leftarrow \mathbf{w} - \nu_k \mathbf{g}$
$k \leftarrow k + 1$
end while

1 Update / 1 forward

Mini-Batch training

Dataset: (X, y) with N samples

Mini-Batch gradient:

Require: Learning rate(s): ν_k
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$k \leftarrow 1$
while stopping criterion not met **do**
Sample m examples $(\mathbf{x}_i, y_i)$ from (X, y)
Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \sum_i^m \nabla_{\mathbf{w}} L(f(\mathbf{x}_i, y_i)$
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  end while

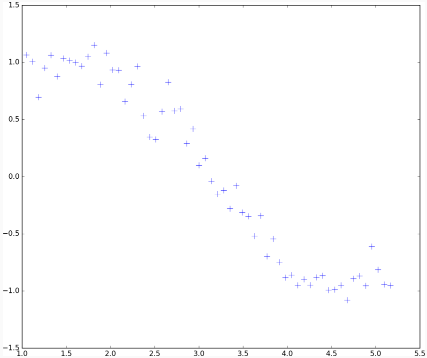
m Update / 1 forward

$m = 1$: Pure stochastic gradient.

$m = N$: Batch gradient

L1/L2 regularization

Example of a non-linear relashonship



An idea

We could take an polynomial hypothesis model:

$$h_{\boldsymbol{\theta}}(x) = \theta_0 x^0 + \theta_1 x^1 + \ldots + \theta_p x^p$$

Example

$\{(x_1, y_1), \ldots, (x_n, y_n)\}$ is the learning dataset.

For a given polynomial degree p, parameters $\boldsymbol{\theta}$ are determined minimizing the least-mean square cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum (y_i - h_{\boldsymbol{\theta}}(x_i))^2$$

with $h_{\boldsymbol{\theta}}(x) = \theta_0 x^0 + \theta_1 x^1 + \ldots + \theta_p x^p$

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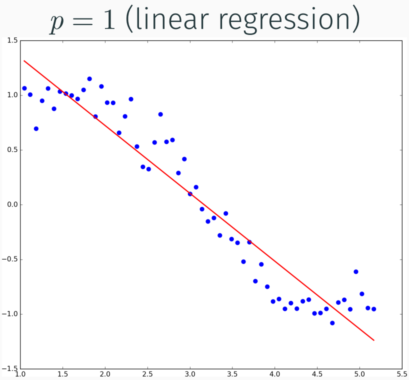
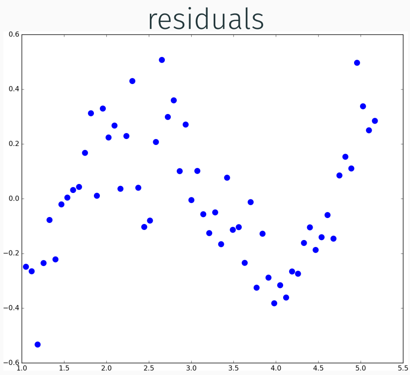
- It can be determined using a gradient descent method
- If the degree of the polynomial $p = 1$, it is a simple linear regression

A first result



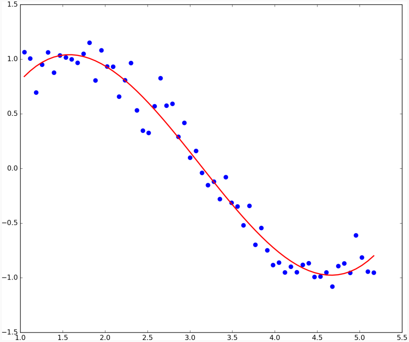


Prediction error

$$\text{err} = \frac{1}{n} \sum \text{res}^2 = 5.46e - 2$$

Increasing the polynomial degree ?

$p = 3$ (cubic regression)



Prediction error

$$\text{err} = \frac{1}{n}\sum \text{res}^2 = 1.80e-2$$

Is it different from the linear regression ?

Let's consider :

$$\boldsymbol{x} = \begin{pmatrix} 1 \\ x^1 \\ x^2 \\ \vdots \\ x^p \end{pmatrix}$$

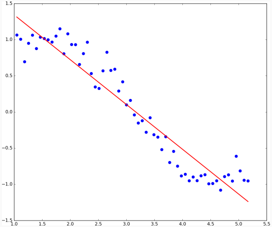
then

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x^1 + \ldots + \theta_p x^p = \boldsymbol{\theta}^T \boldsymbol{x}$$

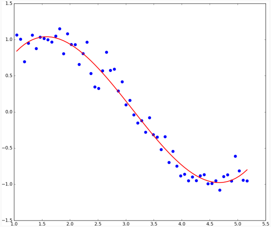
By extending a scalar predictor to a vector, polynomial regression is equivalent to linear regression.

Increasing the degree ?

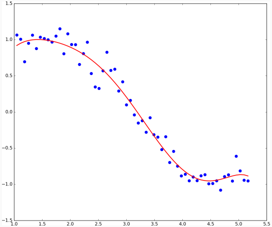
$p = 1$



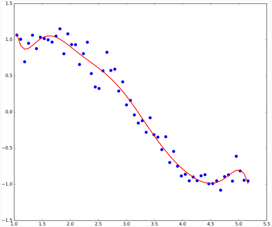
$p = 3$



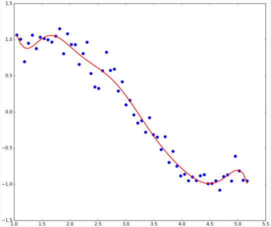
$p = 4$



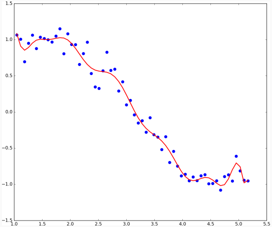
$p = 9$



$p = 12$



$p = 15$



Overfitting

When there is to many paramaters to fit, the model can reproduce a random noise, it is called overfitting

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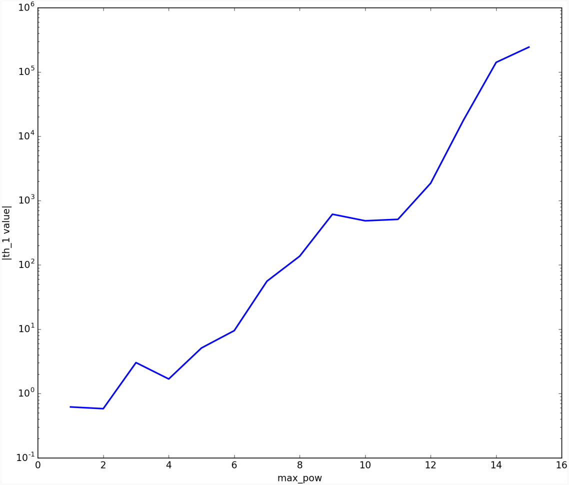
	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
max_pow_1	+5.47e-02	+1.96e+00	-6.20e-01	NaN	NaN	NaN	NaN	NaN	NaN	NaN
max_pow_2	+5.46e-02	+1.91e+00	-5.83e-01	-5.96e-03	NaN	NaN	NaN	NaN	NaN	NaN
max_pow_3	+1.84e-02	-1.08e+00	+3.03e+00	-1.29e+00	+1.37e-01	NaN	NaN	NaN	NaN	NaN
max_pow_4	+1.80e-02	-2.66e-01	+1.69e+00	-5.32e-01	-3.57e-02	+1.39e-02	NaN	NaN	NaN	NaN
max_pow_5	+1.70e-02	+2.99e+00	-5.12e+00	+4.72e+00	-1.93e+00	+3.35e-01	-2.07e-02	NaN	NaN	NaN
max_pow_6	+1.65e-02	-2.80e+00	+9.52e+00	-9.71e+00	+5.23e+00	-1.55e+00	+2.33e-01	-1.36e-02	NaN	NaN
max_pow_7	+1.55e-02	+1.93e+01	-5.60e+01	+6.90e+01	-4.46e+01	+1.65e+01	-3.53e+00	+4.05e-01	-1.92e-02	NaN
max_pow_8	+1.53e-02	+4.32e+01	-1.37e+02	+1.84e+02	-1.33e+02	+5.77e+01	-1.53e+01	+2.42e+00	-2.10e-01	+7.68e-03
max_pow_9	+1.46e-02	+1.68e+02	-6.15e+02	+9.63e+02	-8.46e+02	+4.61e+02	-1.62e+02	+3.68e+01	-5.22e+00	+4.22e-01
max_pow_10	+1.46e-02	+1.38e+02	-4.86e+02	+7.26e+02	-5.96e+02	+2.93e+02	-8.75e+01	+1.45e+01	-8.06e-01	-1.38e-01
max_pow_11	+1.45e-02	-7.49e+01	+5.12e+02	-1.33e+03	+1.87e+03	-1.61e+03	+9.14e+02	-3.50e+02	+9.14e+01	-1.61e+01
max_pow_12	+1.45e-02	-3.39e+02	+1.87e+03	-4.42e+03	+6.01e+03	-5.25e+03	+3.12e+03	-1.30e+03	+3.84e+02	-8.03e+01
max_pow_13	+1.43e-02	+3.20e+03	-1.78e+04	+4.46e+04	-6.66e+04	+6.61e+04	-4.61e+04	+2.32e+04	-8.55e+03	+2.30e+03
max_pow_14	+1.31e-02	+2.38e+04	-1.41e+05	+3.79e+05	-6.10e+05	+6.57e+05	-5.03e+05	+2.82e+05	-1.17e+05	+3.66e+04
max_pow_15	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05

High parameters values

Value of the parameters $|\theta_1|$ with respect with the degree of the polynomial regression



Regularization

The idea

The idea of regularization is to perform a regression minimizing a cost function that includes a term to penalize ”big” values for the parameters:

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum(y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha P(\boldsymbol{\theta})$$

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- Lasso Regularization (L1): $P(\boldsymbol{\theta}) = \sum_{i=0}^{p} |\theta_i|$
- Elastic Net combines both regularization

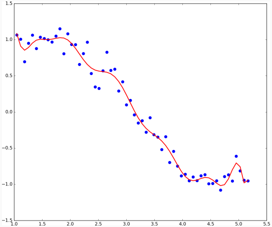
Ridge regression (L2)

Ridge regression is a linear regression with a Ridge regularization:

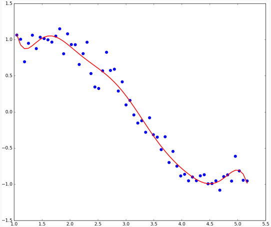
$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum (y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha \sum_{i=0}^{p} \theta_i^2$$

Results for $p = 15$ and varying α

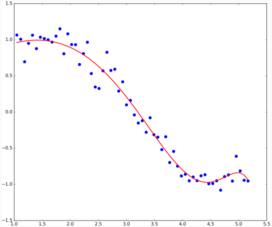
$\alpha = 0$



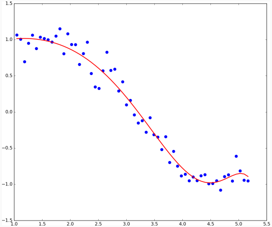
$\alpha = 1e - 15$



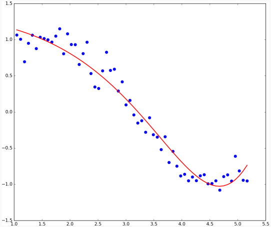
$\alpha = 1e - 4$



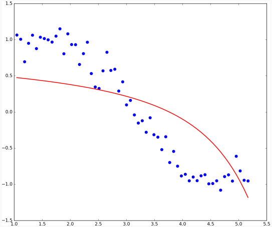
$\alpha = 1e - 3$



$\alpha = 1e - 2$

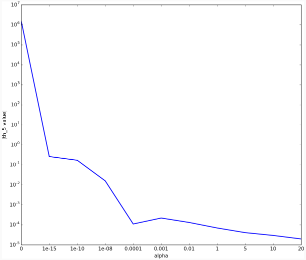


$\alpha = 5$



Values of coefficients

	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
alpha_0	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05
alpha_1e-15	+1.46e-02	+9.43e+01	-2.98e+02	+3.79e+02	-2.37e+02	+6.72e+01	-2.60e-01	-4.35e+00	+5.62e-01	+1.42e-01
alpha_1e-10	+1.54e-02	+1.12e+01	-2.90e+01	+3.11e+01	-1.52e+01	+2.89e+00	+1.69e-01	-9.10e-02	-1.08e-02	+1.98e-03
alpha_1e-08	+1.58e-02	+1.34e+00	-1.53e+00	+1.75e+00	-6.80e-01	+3.88e-02	+1.58e-02	+1.59e-04	-3.60e-04	-5.37e-05
alpha_0.0001	+1.60e-02	+5.61e-01	+5.47e-01	-1.28e-01	-2.57e-02	-2.82e-03	-1.10e-04	+4.06e-05	+1.52e-05	+3.65e-06
alpha_0.001	+1.67e-02	+8.18e-01	+3.05e-01	-8.67e-02	-2.05e-02	-2.84e-03	-2.19e-04	+1.81e-05	+1.24e-05	+3.43e-06
alpha_0.01	+2.39e-02	+1.30e+00	-8.84e-02	-5.15e-02	-1.01e-02	-1.41e-03	-1.32e-04	+7.23e-07	+4.14e-06	+1.30e-06
alpha_1	+9.41e-02	+9.69e-01	-1.39e-01	-1.93e-02	-3.00e-03	-4.66e-04	-6.97e-05	-9.90e-06	-1.29e-06	-1.43e-07
alpha_5	+2.31e-01	+5.48e-01	-5.89e-02	-8.52e-03	-1.42e-03	-2.41e-04	-4.08e-05	-6.87e-06	-1.15e-06	-1.91e-07
alpha_10	+3.00e-01	+4.00e-01	-3.72e-02	-5.53e-03	-9.50e-04	-1.67e-04	-2.96e-05	-5.23e-06	-9.25e-07	-1.63e-07
alpha_20	+3.79e-01	+2.77e-01	-2.25e-02	-3.40e-03	-5.99e-04	-1.08e-04	-1.97e-05	-3.60e-06	-6.58e-07	-1.20e-07



Value of θ_5

Determination of the parameters in the ridge regression

Considering the cost function J:

$$J(\boldsymbol{\theta}) = J_{lms}(\boldsymbol{\theta}) + \alpha \sum_{i=0}^{p} \theta_i^2$$

In a gradient algorithm, update of the parameters:

$\theta_i^{k+1} = \theta_i^k - \nu.(\frac{\partial J_{lms}}{D\theta_i} - 2\alpha\theta_i^k)$

So the update rule is:

$$\theta_i^{k+1} = \theta_i^k(1 - 2\nu\alpha) - \Delta_{lms}$$

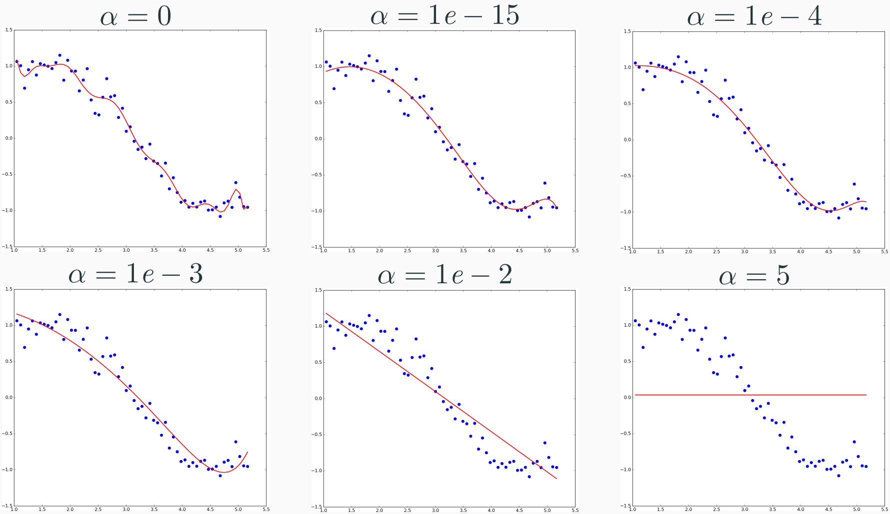
where Δ_{lms} is the update in case of non-regularized regression

Lasso regression (L1)

Lasso regression is a linear regression with a Lasso regularization:

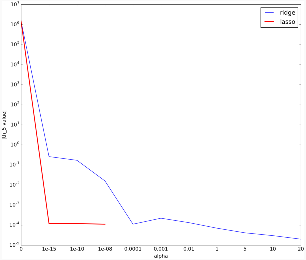
$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum (y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha \sum_{i=0}^{p} |\theta_i|$$

Results for $p = 15$ and varying α



Values of coefficients

	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
alpha_0	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05
alpha_1e-15	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+8.85e-04	+1.63e-03	-1.19e-04	-6.44e-05	-6.28e-06	+1.45e-06
alpha_1e-10	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+8.84e-04	+1.63e-03	-1.18e-04	-6.44e-05	-6.28e-06	+1.45e-06
alpha_1e-08	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+7.69e-04	+1.62e-03	-1.10e-04	-6.45e-05	-6.32e-06	+1.43e-06
alpha_0.0001	+1.72e-02	+9.03e-01	+1.71e-01	-0.00e+00	-4.78e-02	-0.00e+00	-0.00e+00	+0.00e+00	+0.00e+00	+9.47e-06
alpha_0.001	+2.80e-02	+1.29e+00	-0.00e+00	-1.26e-01	-0.00e+00	-0.00e+00	-0.00e+00	+0.00e+00	+0.00e+00	+0.00e+00
alpha_0.01	+6.07e-02	+1.76e+00	-5.52e-01	-5.62e-04	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_1	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_5	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_10	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_20	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00



Value of θ_5

Determination of the parameters in the lasso regression

Considering the cost function J:

$$J(\boldsymbol{\theta}) = J_{lms}(\boldsymbol{\theta}) + \alpha \sum_{i=0}^{p} |\theta_i|$$

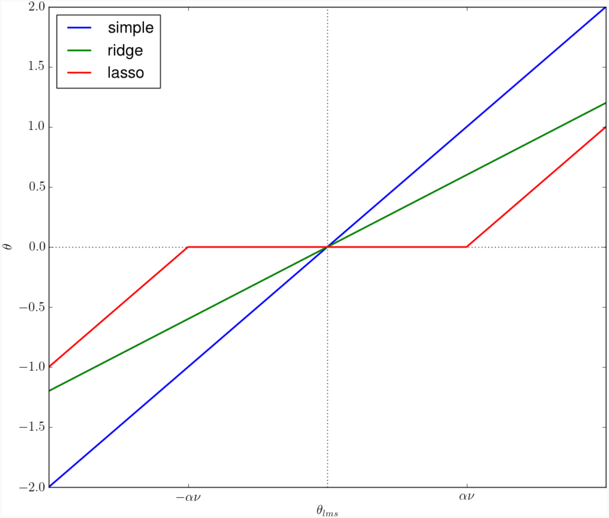
In a gradient algorithm, update of the parameters would be:

J is not differentiable. If we consider $\theta_{lms} = \theta_i^k - \nu.\frac{\partial J_{lms}}{D\theta_i}$

The update rule is:

- $\theta_i^{k+1} = \theta_{lms} + \alpha\nu$ if $\theta_{lms} < -\alpha\nu$
- $\theta_i^k = 0$ if $-\alpha\nu < \theta_{lms} < \alpha\nu$
- $\theta_i^{k+1} = \theta_{lms} - \alpha\nu$ if $\theta_{lms} > \alpha\nu$

Summary of parameters updates



Comparison Ridge/Lasso

Ridge (L2)

- Prevents the overfitting
- includes all the features (dimensions) of the predictor, so it can be useless for high dimensional predictors

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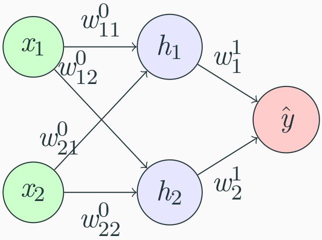
- Prevents the overfitting
- includes all the features (dimensions) of the predictor, so it can be useless for high dimensional predictors

Lasso (L1)

- Provides sparse solutions and reduce the dimension of the predictor
- If some features in the predictor are correlated, arbitrarily select one from the others.

In a neural network

L2 (Ridge) and L1 (Lasso) regularization are widely use in Neural Network architectures.



- Non-regularized loss function: $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2$.
- L2-regularized loss function: $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2 + \alpha \sum_{i=0}^{p} |w_i|$.
- L1-regularized loss function: $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2 + \alpha \sum_{i=0}^{p} w_i^2$.

Wrapping-up

Advantage

L1/L2 regularization prevents overfitting even for large architecture (a big weight vector to optimize)

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Advantage

L1/L2 regularization prevents overfitting even for large architecture (a big weight vector to optimize)

But...

It comes with extra hyperparameter to tune (using, e.g., cross-validation): α

Let’s have a break

`https://playground.tensorflow.org`

Other regularization techniques

Regularization

Definition:

Regularization refers to the set of techniques that constraints the optimization. It is generally used to avoid overfitting, but can also be used to inject prior knowledge during the training phase (e.g. set known limits to parameters)

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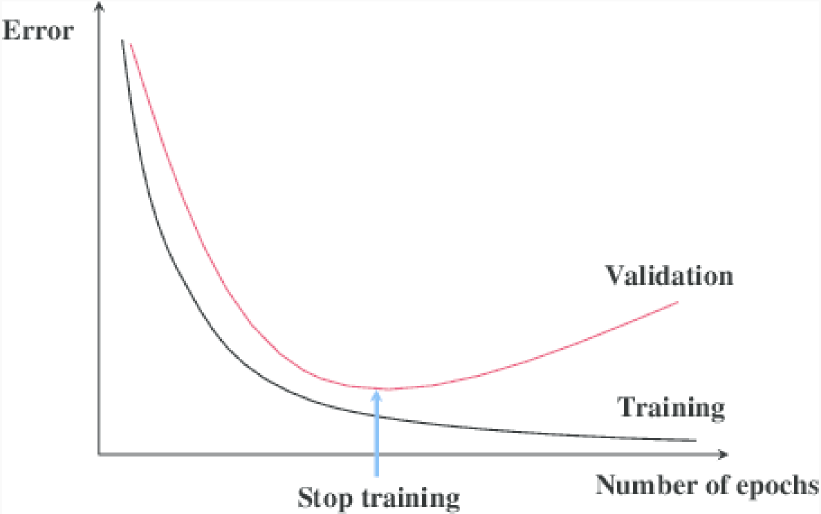
Regularization refers to the set of techniques that constraints the optimization. It is generally used to avoid overfitting, but can also be used to inject prior knowledge during the training phase (e.g. set known limits to parameters)

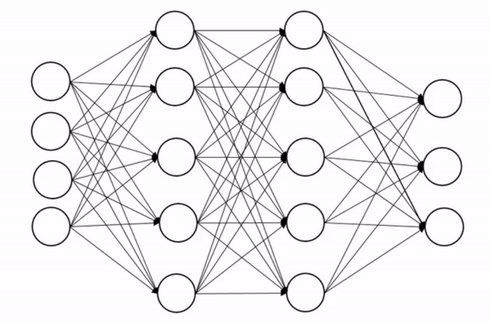
- Stochastic mini-batch gradient is a regularization technique

Early Stopping



Dropout

During training, randomly remove neurons on a layer with probability p.



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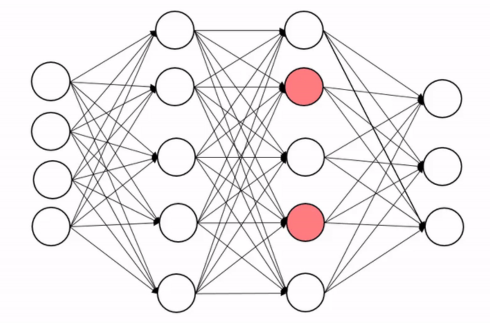

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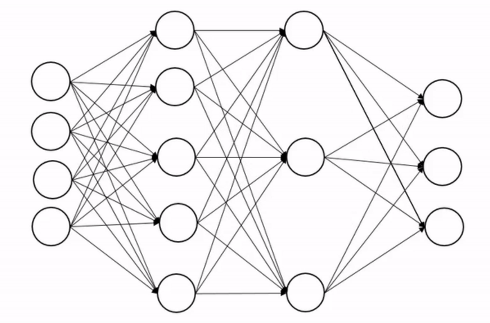

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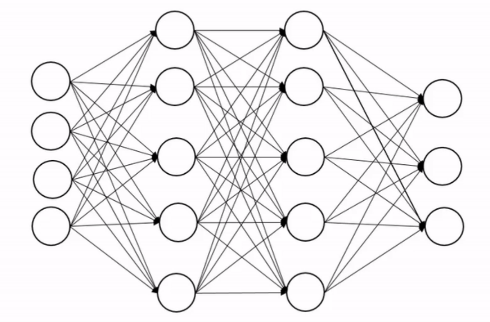

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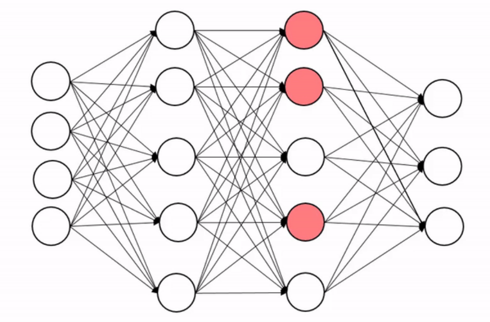

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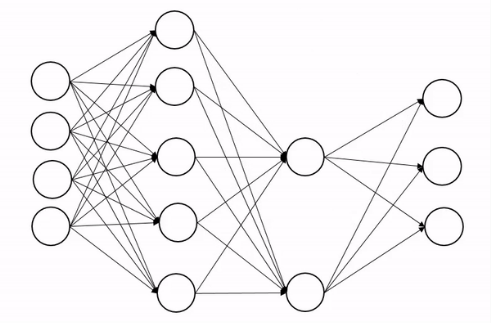

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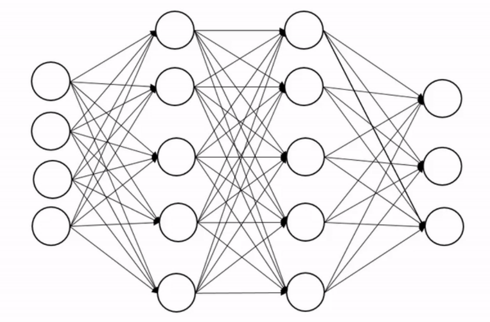

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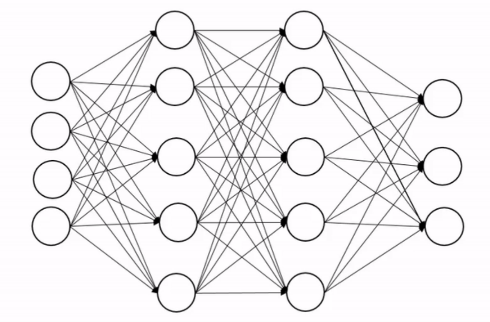

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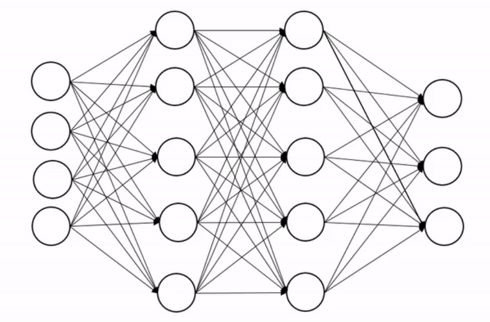

Practical remarks:

- Avoid Dropout on convolutive layer
- Avoid Dropout on the last layer.

Batch normalization

From *Ioffe et al. 2015, Batch normalizaion...*
Batch Normalization is a new type of layer.

If we use mini-batch training with a minibatch of size m:

Mini Batch Layer:

Input: Values of $\mathbf{x_{1\ldots m}}$
Input: Initial parameters to be optimized: γ, β
Output: $\mathbf{z_i} = \mathrm{BN}_{\gamma,\beta}(\mathbf{x}_i)$

$\mu \leftarrow \frac{1}{m}\sum_{i=1}^{m} \mathbf{x}_i$ ▷ mini-batch mean
$\sigma^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (\mathbf{x}_i - \mu)^2$ ▷ (mini-batch variance)
$\hat{\mathbf{x}}_i \leftarrow (\mathbf{x}_i - \mu)/\sqrt{\sigma^2 + \epsilon}$ ▷ normalize
$\mathbf{z_i} = \gamma\hat{\mathbf{x}}_i + \beta$ ▷ Scale and shift
return $\mathbf{z_i}$

μ and σ^2 are non-trainable parameters. They are fixed for inferring new result (in test/validation).

Link with data assimilation

Example of BLUE: Best Linear Unbiased Estimator

Given a state vector $\mathbf{x} \in \mathbb{R}^n$ and a data vector $\mathbf{d} \in \mathbb{R}^m$:

$$\mathbf{x}^{\mathrm{f}} = \mathbf{x}^{\mathrm{t}} + \mathbf{p}, \qquad \overline{\mathbf{p}} = 0, \qquad \overline{\mathbf{p}\mathbf{p}^T} = \mathbf{C}_{xx}.$$

$$\mathbf{d} = \mathbf{H}\mathbf{x}^{\mathrm{t}} + \boldsymbol{\epsilon}, \qquad \overline{\boldsymbol{\epsilon}} = 0, \qquad \overline{\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T} = \mathbf{C}_{\epsilon\epsilon}.$$

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Estimating $\mathbf{x}^{\mathrm{t}}$ by minimizing the estimation error leads to minizing the following function:

$$\mathcal{J}(\mathbf{x}) = (\mathbf{d} - \mathbf{H}\mathbf{x})^T \mathbf{C}_{\epsilon\epsilon}^{-1} (\mathbf{d} - \mathbf{H}\mathbf{x}) + (\mathbf{x} - \mathbf{x}^{\mathrm{f}})^T \mathbf{C}_{xx}^{-1} (\mathbf{x} - \mathbf{x}^{\mathrm{f}})$$

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This is data assimilation!

We correct a forecast $\mathbf{x}^{\mathrm{f}}$ given some observational data $\mathbf{d}$

Is it machine learning?

- Ridge regression: $J(\boldsymbol{\theta}) = (\mathbf{y} - h_{\boldsymbol{\theta}}(\mathbf{x}))^T(\mathbf{y} - h_{\boldsymbol{\theta}}(\mathbf{x})) + \alpha\theta^T\theta$
- BLUE: $\mathcal{J}(\mathbf{x}) = (\mathbf{d} - \mathbf{H}\mathbf{x})^T\mathbf{C}_{\epsilon\epsilon}^{-1}(\mathbf{d} - \mathbf{H}\mathbf{x}) + (\mathbf{x} - \mathbf{x}^{\mathrm{f}})^T\mathbf{C}_{xx}^{-1}(\mathbf{x} - \mathbf{x}^{\mathrm{f}})$

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BLUE	Ridge
data $\mathbf{d}$	target $\mathbf{y}$
Observation operator $\mathbf{H}$	feature $\mathbf{x}$
State $\mathbf{x}$	parameters $\boldsymbol{\theta}$
$\mathbf{C}_{\epsilon\epsilon}\mathbf{C}_{xx}^{-1}$	α

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- BLUE: $\mathcal{J}(\mathbf{x}) = (\mathbf{d} - \mathbf{H}\mathbf{x})^T\mathbf{C}_{\epsilon\epsilon}^{-1}(\mathbf{d} - \mathbf{H}\mathbf{x}) + (\mathbf{x} - \mathbf{x}^{\mathrm{f}})^T\mathbf{C}_{xx}^{-1}(\mathbf{x} - \mathbf{x}^{\mathrm{f}})$

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Further links...

If a numerical model is integrated over several time steps, it can be related to successive layers of a Neural Network.

Questions addressed in this lecture

- What is gradient backpropagation? [GBC16,6]
- What are the different types of gradient descent techniques? [GBC16,8]
- What is L1(Lasso)/L2(Ridge) regularization? [Van16,5.6; GBC16,8]
- What are some other types of regularizations? [GBC16,7]
- How machine learning can be related to data assimilation?
- Who is going to win the next Rugby world cup?

Refs

[Van16,n]: Jake VanderPlas, *Python Data Science Handbook*, section n
[GBC16,n]: Goodfellow etal., Deep Learning, chapter n