Training ML models

Cambridge ICCS summer school

cambridge-iccs.github.io/summerschool

Will Handley

2022-09-22

Slides & installation instructions at

`https://github.com/handley-lab/2022-cambridge-iccs`

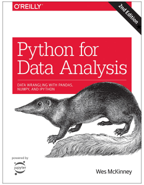
Overview

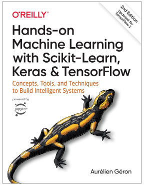
- Title is rather broad, and we have < 2h, the morning after the conference dinner.
- Aim to build a framework of understanding in the context of a few examples
- Should be able to answer:
  - What is an ML model?
  - How do I avoid pitfalls in training them?
  - Which resources should I reach for in the future?

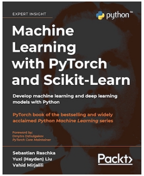
The Machine Learning Python stack

0. `numpy`
   - Layer zero – vector maths & array-based programming
   - Advanced users: broadcasting, `x @ y`, `z[:,None]`, ufuncs
1. `scipy` & `pandas`
   - Extends `numpy` to numerical algorithms and excel-like array functionality
   - `pandas` often a data scientist’s weakest point
2. `scikit-learn`
   - Entry-level machine learning
   - Extends to allow estimators, transformers & predictors
   - With a few key concepts this is a consistent and versatile ML framework
3. `Keras`/`TensorFlow` `PyTorch`,
   - Deep learning tools
   - Familiarity with the previous layers greatly enhances effectiveness

+ `matplotlib` for plotting (others exist, extending and reducing flexibility)



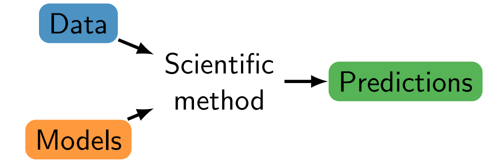

O'REILLY
2nd Edition Updated for TensorFlow 2
Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow
Concepts, Tools, and Techniques to Build Intelligent Systems
powered by jupyter
Aurélien Géron


EXPERT INSIGHT
python
Machine Learning with PyTorch and Scikit-Learn
Develop machine learning and deep learning models with Python
PyTorch book of the bestselling and widely acclaimed Python Machine Learning series
Foreword by: Dmytro Dzhulgakov PyTorch Core Maintainer
Sebastian Raschka
Yuxi (Hayden) Liu
Vahid Mirjalili
Packt

What is machine learning?

What is machine learning?

- A computer program which can program itself to perform a task
  - Problems with lots of tuning/rules
  - Problems with no traditional solution
  - Fluctuating environments
  - Gaining insight about complex data
- Traditional programs
  - Quicksort
  - Pong
- Machine learning
  - Spam filter
  - Netflix suggestions
  - Speech recognition
  - Dall-E

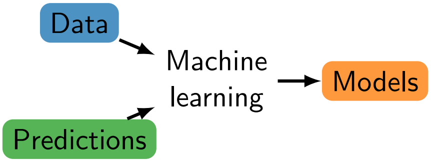


Data

Models

Scientific method

Predictions



Data

Predictions

Machine learning

Models

The machine learning pipeline

1. Problem framing
2. Data acquisition
3. Visualisation
4. Data preparation/munging
5. Selecting & training a model
6. Tuning a model
7. Launch, monitor & maintain

The machine learning pipeline

1. Problem framing
   - Big picture
   - Selecting performance measures/objectives
   - Checking assumptions/bias
2. Data acquisition
3. Visualisation
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The machine learning pipeline

1. Problem framing
2. Data acquisition
   - Gather your data
   - Selecting performance measures/objectives
   - Checking assumptions/bias
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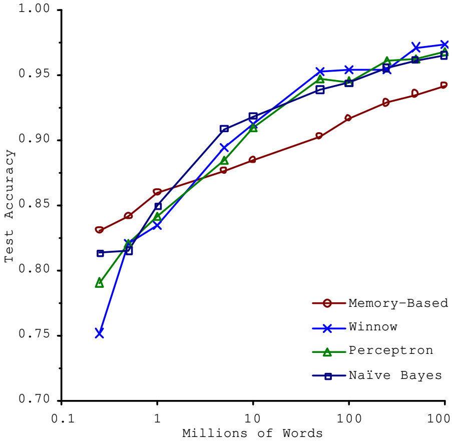

[doi:10.3115/1073012.1073017]

The machine learning pipeline

1. Problem framing
2. Data acquisition
3. Visualisation
    - using pandas+matplotlib skills to explore ideosyncrasies of the data
4. Data preparation/munging
5. Selecting & training a model
6. Tuning a model
7. Launch, monitor & maintain

The machine learning pipeline

1. Problem framing
2. Data acquisition
3. Visualisation
4. Data preparation/munging
   - using scikit-learn to clean & transform the data
5. Selecting & training a model
6. Tuning a model
7. Launch, monitor & maintain

The machine learning pipeline

1. Problem framing
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5. Selecting & training a model
    - Topic of this session
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The machine learning pipeline

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The machine learning pipeline

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2. Data acquisition
3. Visualisation
4. Data preparation/munging
5. Selecting & training a model
6. Tuning a model
7. Launch, monitor & maintain
    - For researchers this could be github distributing
    - For industry this would mean real-world shipping

Categories of machine learning

Supervised

Regression
Classification

Unsupervised

Clustering, Visualisation, Dimensionality reduction

Semisupervised

Google Photos

Reinforcement

AlphaGo, GANNS

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Offline learning using all available data.

Online

Training/updating on-the-fly on mini-batches, for memory-bound/out-of-core

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Instance based learning

"Learn-by-heart" – given a similarity measure, compare/regress/classify new examples onto existing data

Model-based learning

Build a parameterised model of data, train it, then make predictions

Challenges of Machine Learning

- Bad data
  - Not enough
  - Not representative
  - Poor quality (outliers, noise)
  - Irrelevant/Poor features
- Bad algorithm/Bad training (Focus of this workshop)
  - Overfitting
  - Underfitting

Example 1: Introduction to regression

Slides & installation instructions at
`https://github.com/handley-lab/2022-cambridge-iccs`

Training an ML model

- Three ingredients to training
  1. Input data/features $\boldsymbol{x}^{(i)}$, output data $y^{(i)}$, where $i = 1, \ldots n_{\text{obs}}$
  2. Parameterised model $\boxed{y = h_{\boldsymbol{\theta}}(\boldsymbol{x})}$, where h is the model and $\boldsymbol{\theta}$ are its parameters
  3. Loss function(s) $L(y_{\text{pred}}, y)$
- Train the parameters on a training subset by solving the mathematical problem

$$\hat{\boldsymbol{\theta}} = \min_{\boldsymbol{\theta}} \sum_{i \in \text{train}} L_{\text{train}} \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)} \right)$$

- Choose the best model by minimising a (possibly different) loss on a validation subset

$$\hat{h} = \min_{h} \sum_{i \in \text{validation}} L_{\text{validation}} \left(h_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}^{(i)}), y^{(i)} \right)$$

- Finally test the best model on set-aside testing data.

1. Data

- The initial data $\{(\boldsymbol{x}^{(i)}, y^{(i)}), i = 1, \ldots, n_{\text{obs}}\}$ must usually be transformed
- Relevant features should be selected
- Relevant combinations of features should be considered (e.g. computing rates/sums)
- This is known as feature engineering
- Features should then be normalised, Either:

  min-max scaled data lie in $[0, 1]$ (`sklearn.preprocessing.MinMaxScaler`)
  standardised data have mean 0 and std 1 (`sklearn.preprocessing.StandardScaler`)
- The `sklearn` way to do this is to chain a set of these transformations together in a `sklearn.pipeline.Pipeline`
- This is essential since almost all machine learning algorithms are not covariant, and will fail on unnormalised data.

2. Models

- "How to choose models" would fill a whole other session.
- You may recognise some of the standard choices.
- Models have trainable parameters $\boldsymbol{\theta}$, and hyperparameters.

Supervised

- k-Nearest Neighbors
- Linear Regression
- Logistic Regression
- Support Vector Machines
- Decision Trees and Random Forests
- Neural Networks

Semisupervised

- deep belief networks
- RBMs

Reinforcement

- AlphaGo
- GANNs

Unsupervised

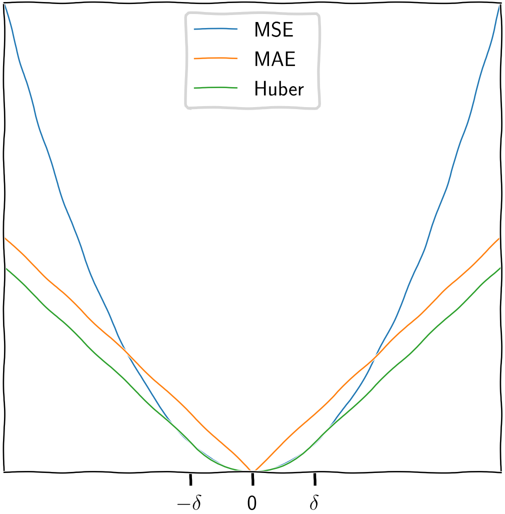
- Clustering
  - K-Means
  - DBSCAN
  - Hierarchical Cluster Analysis
- Anomaly detection
  - One-class SVM
  - Isolation forest
- Visualisation and dimensionality reduction
  - (Kernel) PCA
  - Locally-Linear Embedding
  - t-SNE
- Association rule learning
  - Apriori & Eclat

3. Loss functions

- All that is needed is something which measures how "close" a model's prediction is to the true answer
- The loss function you train on does not need to be the same as the testing/validation metric.
- Mean square error (MSE) $L = (\Delta y)^2$
  - smooth (differentiable)
- Mean absolute error (MAE) $L = |\Delta y|$
  - robust to outliers
- Huber loss

$$L = \begin{cases} \frac{1}{2}(\Delta y)^2 & |\Delta y| < \delta \\ \delta((\Delta y) - \frac{1}{2}\delta) & |\Delta y| >= \delta \end{cases}$$

  - combines benefits of both



Principles of Training, Validation & Testing splits

- The sure-fire way to know how a model will generalise is to hold back data for testing.
- We therefore split data into three categories

Training

∼80% of the data.
Used for learning parameters.

+Validation

Used for learning hyperparameters.

Testing

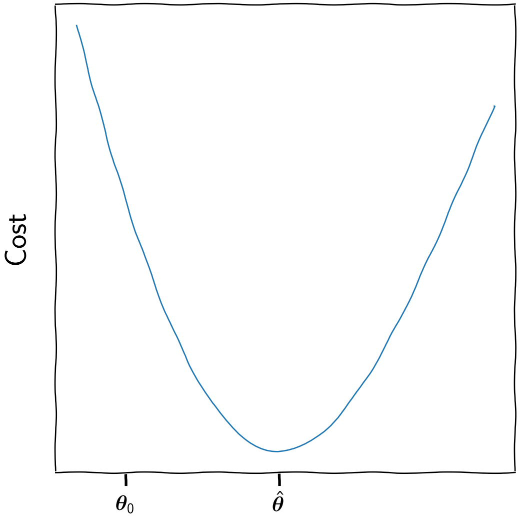
Holdout ∼20% of the data.
Should be ideally "one-shot".

- "Validation set" is also known as the "development/dev set".
- If we do repeated holdout validation on many small validation sets, this is cross-validation.
- Gotchas:
  - standardisation/data preparation should only use the training+validation set
    - Failing to do this reduces generalisability
  - ideally the splitting procedure should be random, but seedable
    - Failing to do this reduces repeatability & reliability
  - `sklearn.model_selection.StratifiedKFold` accomplishes these and more

Gradient descent

- To minimise a function $f(\boldsymbol{\theta})$, start somewhere $\boldsymbol{\theta}_0$ and go downhill (down the gradient) by some step η

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta})$$



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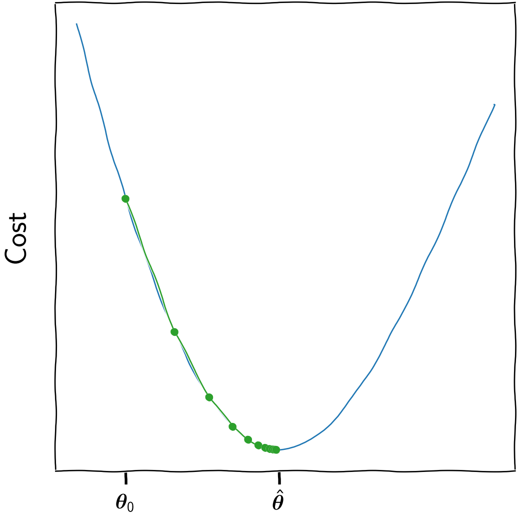

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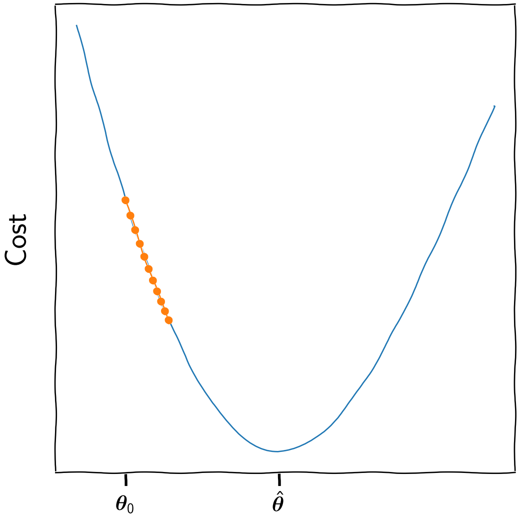
- Problems:
  - Learning rate too slow



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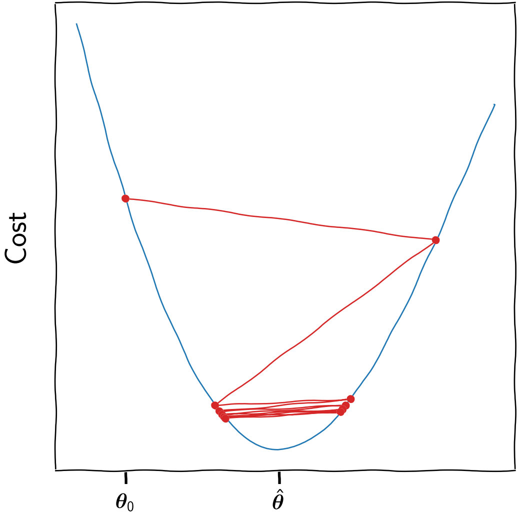
- Problems:
  - Learning rate too slow
  - Learning rate too fast



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  - Learning rate too slow
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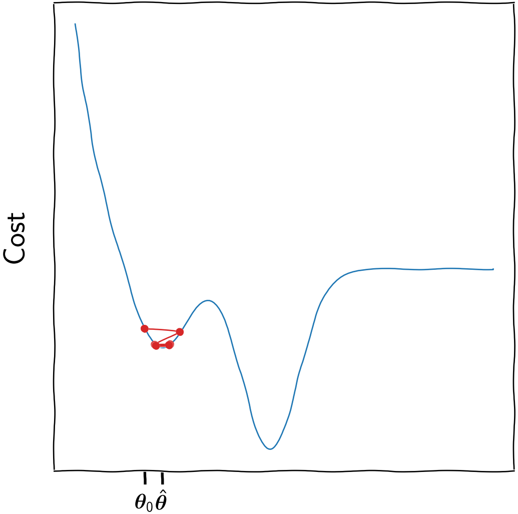

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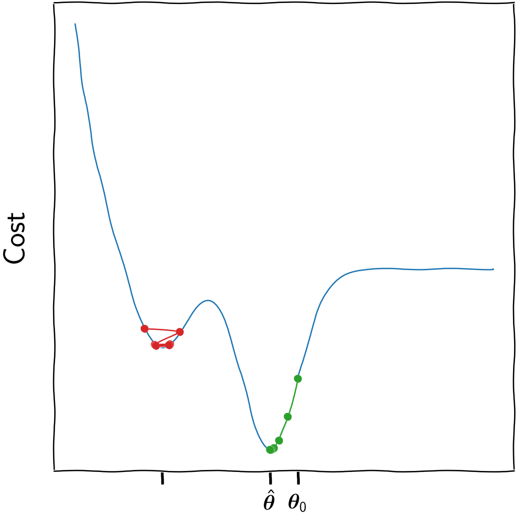

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- Problems:
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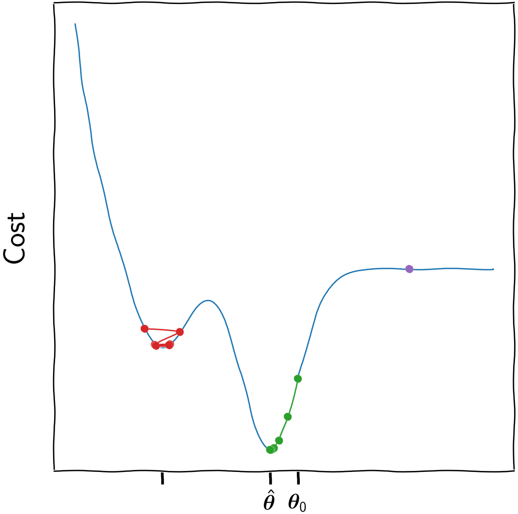
  - Learning rate too fast
  - Local minima
  - stalling



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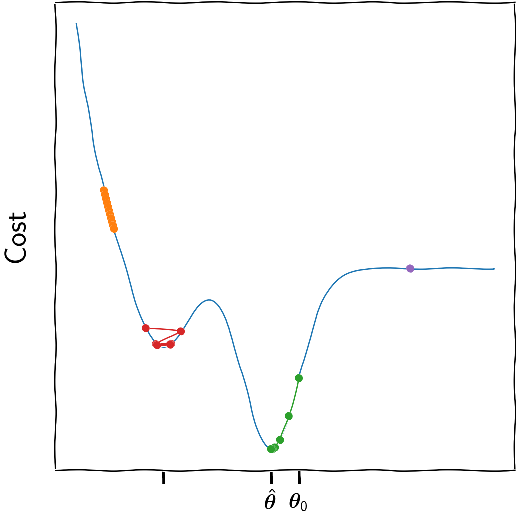
- Problems:
  - Learning rate too slow
  - Learning rate too fast
  - Local minima
  - stalling
- Choosing the learning rate, or more generally tuning the learning schedule can be the hardest part of training.
- All much harder in higher dimensions



Example 2: Machine learning with scikit-learn

Go back to the notebook `training_ml_models.ipynb`

For more detail on the scikit-learn API (beyond the docs) I recommend [arxiv:1309.0238]

How we get the gradients: autodiff

- There are three ways to get a computer to compute a gradient $\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta})$
  1. Analytically
     - Painstakingly coding the function explicitly
     - Accurate, but practically impossible for all but the simplest functions
  2. Numerically
     - Computing finite differences $[\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta})]_i \approx [f(\boldsymbol{\theta} + \delta\, \hat{\boldsymbol{e}}_i) - f(\boldsymbol{\theta})]\,/\delta$
     - Easy, but prone to numerical instability
     - Expensive – costs $\sim \mathcal{O}(n)$ function evaluation for each coordinate direction $\hat{\boldsymbol{e}}_i$
  3. Automatically
     - Every computer programme is composed of logic, multiplication and addition.
     - A smart enough computer, equipped with a chain rule, can therefore differentiate any code.
     - Remarkably, this can be done at the same cost as computing f
- Autodiff has been around for a long time, but unless the programmming language is designed with it in mind it is difficult in practice.
- Modern ML codes are.
- In traditional ML literature this is wrapped up in a mythology of "backpropagation" – equivalent to "reverse mode autodiff", well suited to high-chaining with few outputs.

Variations on gradient descent

Batch gradient descent (full)

Compute the gradient in full at each step:

$$\nabla_{\boldsymbol{\theta}} \sum_i \left[L(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)}) \right]$$

Deterministic.
Slow for large data sets.

Stochastic gradient descent (SGD)

Compute the gradient on one random data point

$$\nabla_{\boldsymbol{\theta}} \left[L(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(j)}), y^{(j)}) \right]$$

Blazingly fast.
Randomness can escape minima.

Mini-batch gradient descent

Compute the gradient on a (small) subset of points

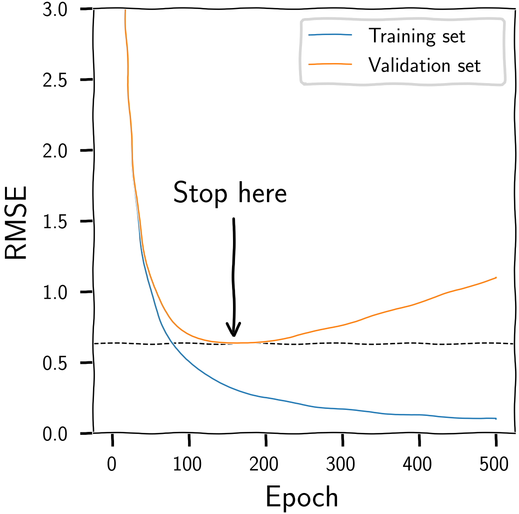
$$\nabla_{\boldsymbol{\theta}} \sum_{i \in \text{batch}_j} \left[L(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)}) \right]$$

GPU accelerable.
Batch size < 32.

- In addition SGD & mini-batch have benefits for out-of-core learning, when the data are too large to fit into memory.

Regularisation

- Can reduce overfitting by constraining the degrees of freedom of the model
  - reduce the number of free parameters
  - constrain the parameters to a reduced range
- Regularisation (only applied at training)
  - Ridge regression: $L(\boldsymbol{\theta}) + \frac{1}{2}\alpha\sum_i \theta_i^2$
  - Lasso regression: $L(\boldsymbol{\theta}) + \alpha\sum_i |\theta_i|$
    - Least absolute shrinkage & selection operator
    - Promotes sparsity
  - Elastic Net: $L(\boldsymbol{\theta}) + r\alpha\sum_i |\theta_i| + \frac{1-r}{2}\alpha\sum_i \theta_i^2$
- Early stopping
  - Halt training when validation error increases.
  - As close to a free lunch as one gets.
  - Very popular.



Neural networks

A multi-layer perceptron (MLP) is mathematically

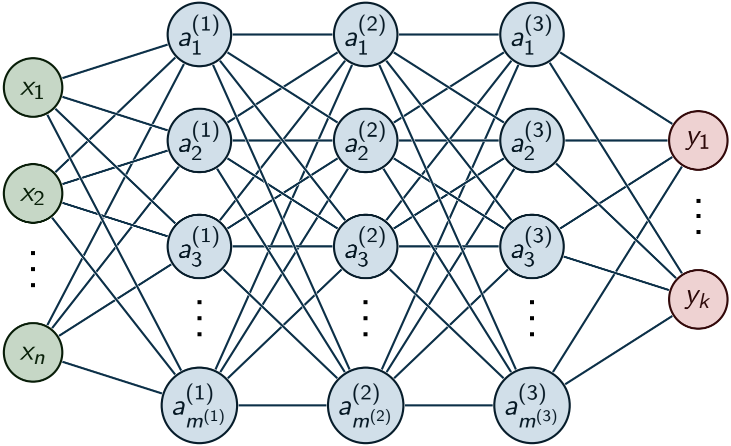
$$a_i^{(\ell+1)} = \phi_i^{(\ell)}\left(\sum_{j=1}^{m^{(\ell)}} w_{ij}^{(\ell)} a_j^{(\ell)} + b_i^{(\ell)}\right)$$

or written in vectors:

$$\boldsymbol{a}^{(\ell+1)} = \boldsymbol{\Phi}^{(\ell)}\left(\boldsymbol{W}^{(\ell)}\boldsymbol{a}^{(\ell)} + \boldsymbol{b}^{(\ell)}\right)$$

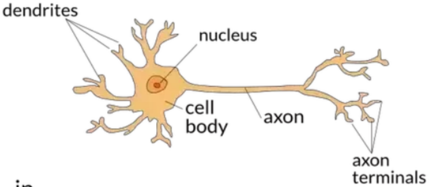
$$\boldsymbol{a}^{(0)} = \boldsymbol{x}, \qquad \boldsymbol{y} = \boldsymbol{a}^{(m+1)}$$

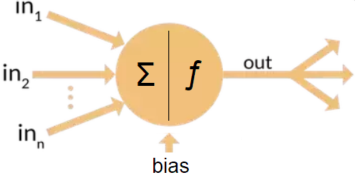
or graphically:

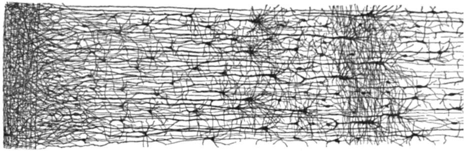


Neural networks & “deep” learning

- NNs were originally inspired by biology.
- Old technology (1960s), came of age in 1990s.
  - rise in computing power
  - innovations in training
  - funding/interest from tech companies
- Universal approximation theorem:
  Any function $\mathbb{R}^n \to \mathbb{R}^k$ can be approximated by a sufficiently wide single hidden layer NN
- So why do we need “deep” (multi-layer) networks?
- Earlier layers perform feature learning to pipe into final universal approximating layer
- Enables the rudiments of transfer learning







Deep learning tools

TensorFlow (Google/Alphabet)

- 2015
- Symbolic math library
- Keras makes easier
- More popular in industry

PyTorch (Facebook/Meta)

- 2017
- Easier to get started
- Faster than Keras
- More popular in research

- Keras is a Python API to TensorFlow, CNTK & Theano
- CNTK is MicroSoft's (now defunct) "cognitive toolkit"
- Theano used to be a giant in the field, and is a 2007 "grandfather" to the rest. Now only used by research/legacy code

In summary: the big boys & girls in industry use TensorFlow, but since PyTorch is preferred and developed by research now, it may become dominant in a few years time. Keras is a wrapper to TensorFlow which makes it more native, but slower and less flexible

Neural Network Anatomy & Training

The dials you can twiddle

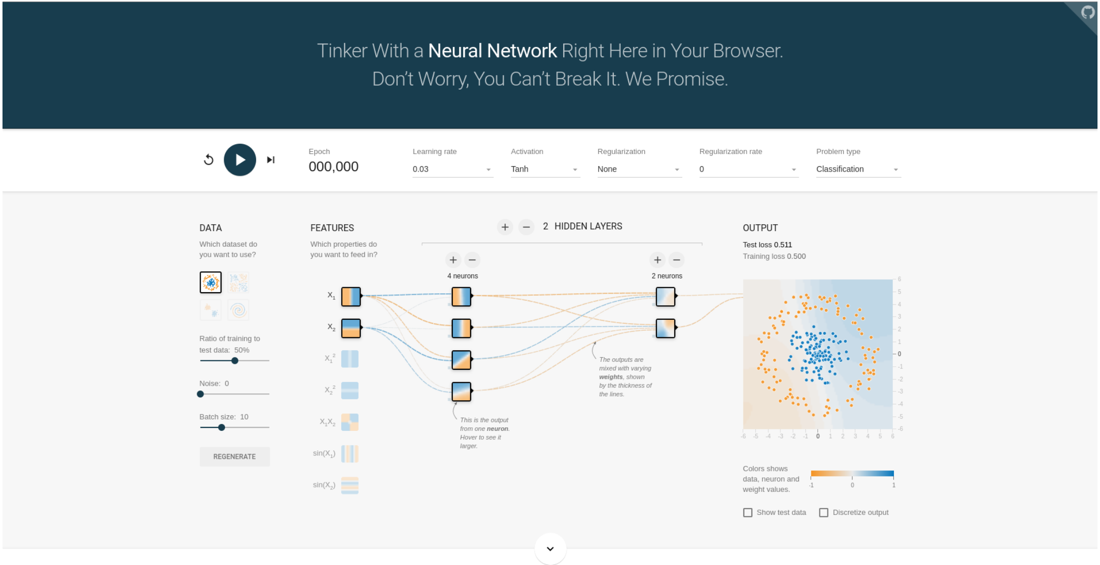
Anatomy

- Number of hidden layers
- Width of hidden layers
- Activation functions

Training

- Loss function
- Optimiser
- Initialisation
- Normalisation
- Regularisation
- Learning rate schedule

playground.tensorflow.org



Tinker With a **Neural Network** Right Here in Your Browser.
Don't Worry, You Can't Break It. We Promise.

Epoch 000,000

Learning rate 0.03

Activation Tanh

Regularization None

Regularization rate 0

Problem type Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

REGENERATE

FEATURES

Which properties do you want to feed in?

2 HIDDEN LAYERS

4 neurons

2 neurons

*This is the output from one **neuron**. Hover to see it larger.*

*The outputs are mixed with varying **weights**, shown by the thickness of the lines.*

OUTPUT

Test loss 0.511

Training loss 0.500

Colors shows data, neuron and weight values.

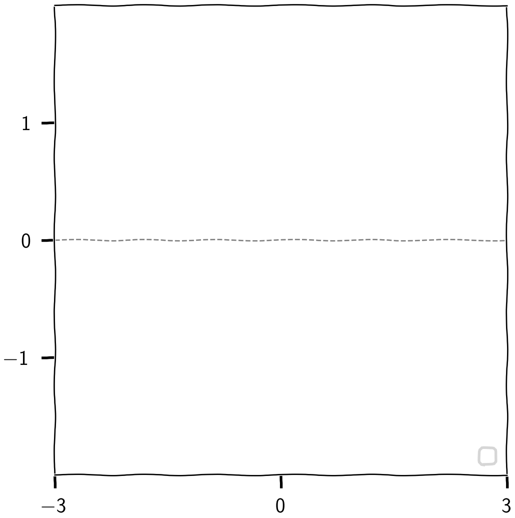
□ Show test data □ Discretize output

Hyperparameter tuning

- The amount of things you can change in a neural network is both an advantage and the main drawback
- Coming up with new combinations forms a thriving field in itself
- There are some automated tools for hyperparameter tuning beyond the cross-validation grids we've found before
  - Hyperopt (Python)
  - Hyperkeras, kopt or talos (Keras)
  - Scikit-Optimise (e.g. `BayesSearchCV`)
  - Spearmint (more Bayesian optimisation)
  - Sklearn-Deap (evolutionary algorithms)
  - . . .
- There are also cloud computing services (Google Cloud, Arimo, SigOpt, Oscar,. . .)
- Finding a more principled way to choose these parameters is a big unsolved problem.
- Nevertheless, there are still some principles which are helpful to know

Activation functions

- There is now a veritable zoo of activation functions
- Important properties to consider:
  - Smoothness
  - Saturation (at either end)
- Different roles depending on layer
  - At output it is useful to e.g. impose positivity with softmax or [0,1] boundedness with logistic
  - For inner layers one may want symmetry/infinite range



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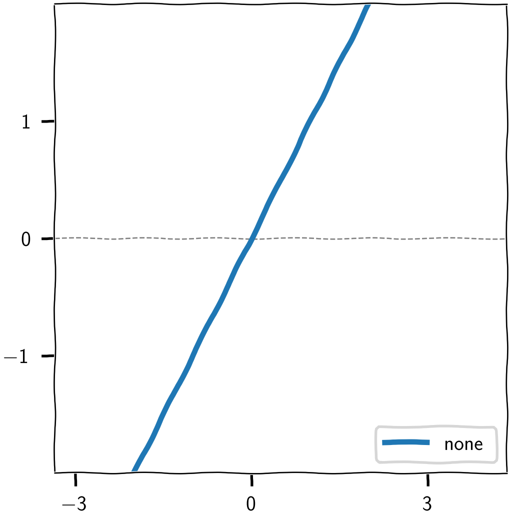

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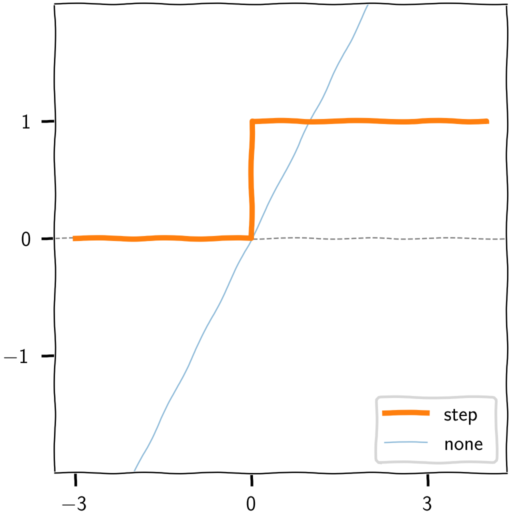
  - At output it is useful to e.g. impose positivity with softmax or [0,1] boundedness with logistic
  - For inner layers one may want symmetry/infinite range



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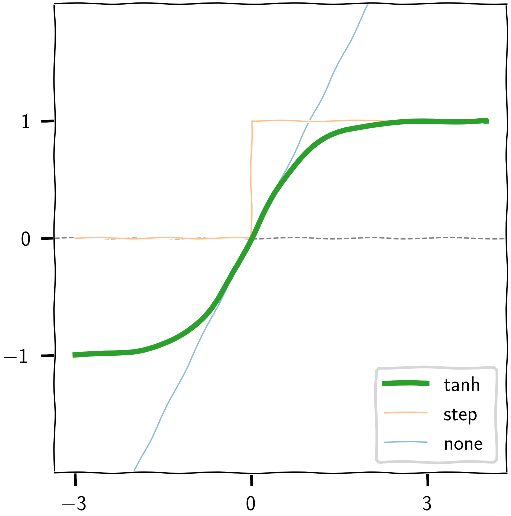

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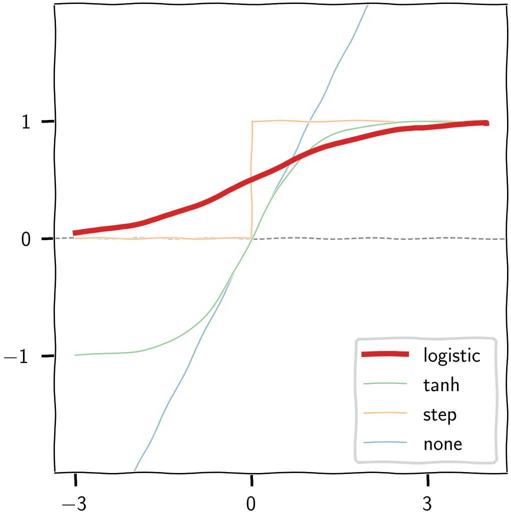

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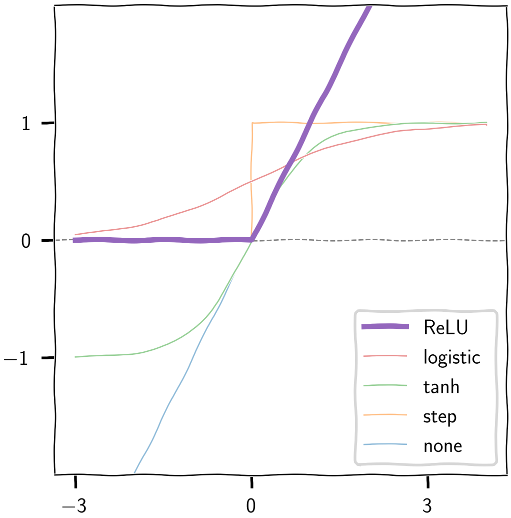

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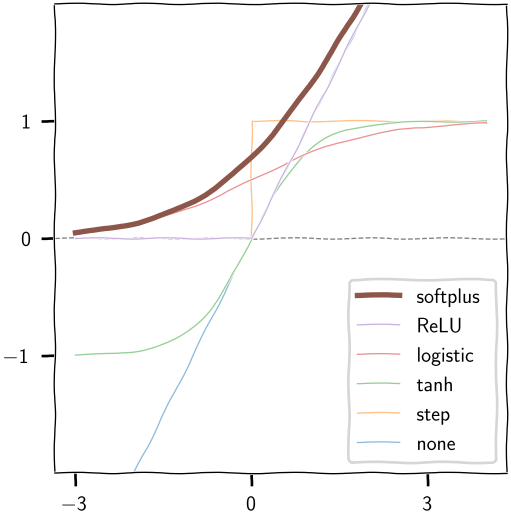

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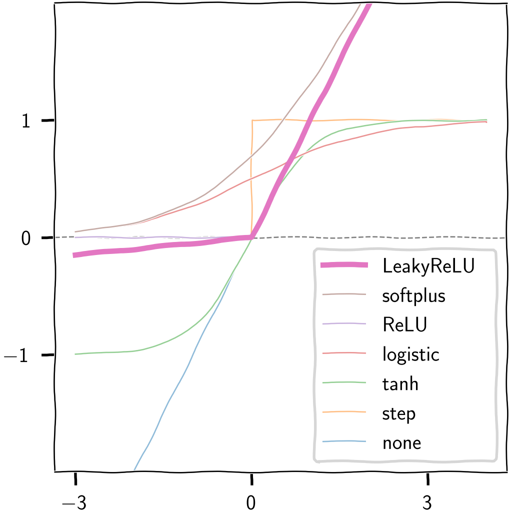

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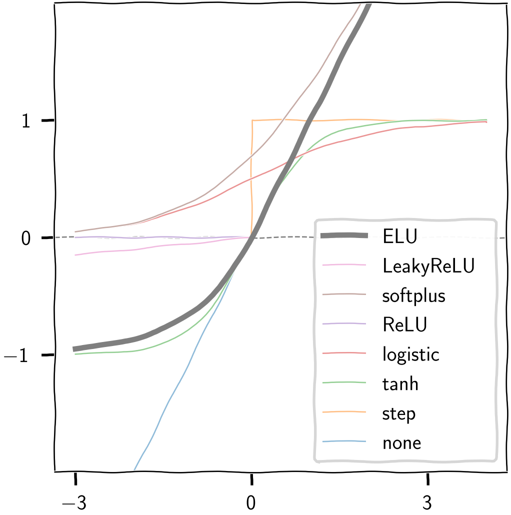

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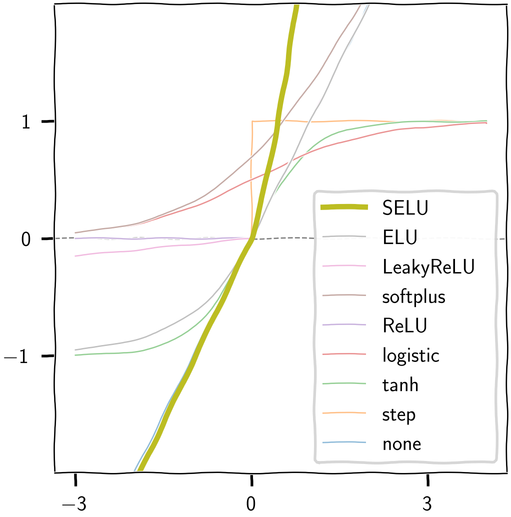

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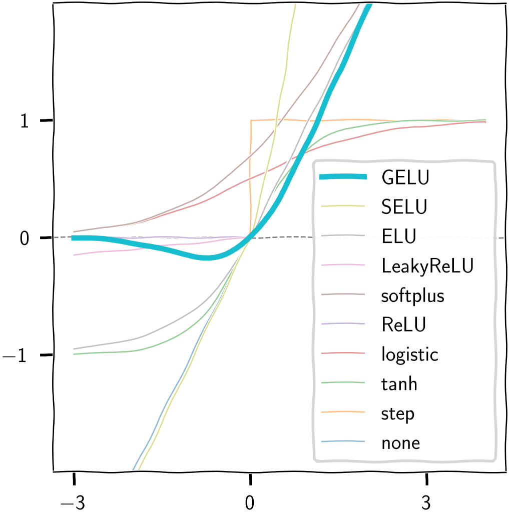


Typical architectures

All problem dependent, but some reasonable guidelines are

Regression

# input neurons	1 per input feature
# hidden layers	1 to 5
# neurons per hidden layer	Typically 10 to 100
# output neurons	1 per output dimension
Hidden activation	ReLU (or SELU)
Output activation	None
(positive outputs)	ReLU/Softplus
(bounded outputs)	Logistic/Tanh
Loss function	MSE
(if outliers)	MAE/Huber

Classification

Same as Regression, except

- Loss function: cross-entropy
- # output neurons: same as number of labels/classes
- Output layer activation: Logistic for binary classifications and softmax for multiclass.

Number of hidden layers

- Often a single layer will do (UAP)
- Deep networks allow you to do feature learning in the earlier layers
- This also enables transfer learning
- Start with one or two hidden layers, and gradually ramp up until you start overfitting.
- It may be helpful to use pre-trained networks

Width of hidden layers

- Historically we “ramped down”, e.g. starting with 300, then 200, then 100
- In practice this makes little difference and adds tuning parameters
- Rectangular networks therefore more common
- Start with a small number and ramp up until the model starts overfitting

Building neural networks

- Sequential API
  - Straightforward models
- Functional API
  - Complicated models
- Subclassing API
  - Dynamic models

Example 3: Training Neural Networks

Go back to the notebook `training_ml_models.ipynb`

Difficulties in training deep networks

- Exploding/vanishing gradients
- Not enough training
- Slow training
- Overfitting due to to many parameters

Vanishing/Exploding gradients: weight initialisation

- Gradients vanish at plateaus, and explode if able to grow without bound (more common in recurrent neural networks)
- A step-change improvement in performance can be found by weight initialisation ($\boldsymbol{\theta}_0$)
- Standard normally distributed (mean 0 variance 1) weights piped into an activation function do not result in mean 0 variance 1 outputs.
- A standard initialised network starts from a point of saturation.
- Terminology: $\mathrm{fan}_{\mathrm{avg}} = \frac{1}{2}(\mathrm{fan}_{\mathrm{in}} + \mathrm{fan}_{\mathrm{in}})$, where $\mathrm{fan}_{\mathrm{in}} \equiv$ circuit terminology to describe the number of inputs to a layer

Glorot

Activation: None, Tanh, logistic, softmax.
initialise weights: Normal with variance
$\sigma^2 = \frac{1}{\mathrm{fan}_{\mathrm{avg}}}$ (or Uniform in $\pm\sqrt{3/\mathrm{fan}_{\mathrm{avg}}}$)

He

Activation: ReLU *et al.*
initialise weights:
variance $\sigma^2 = \frac{2}{\mathrm{fan}_{\mathrm{in}}}$

Lecun

Activation: SELU
initialise weights:
variance $\sigma^2 = \frac{1}{\mathrm{fan}_{\mathrm{in}}}$

Vanishing/Exploding gradients: Nonsaturating activation functions

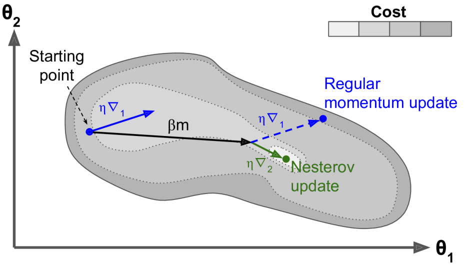
- Another way to fix the saturation problem is to choose a nonsaturating activation function (N.B. This is not how mother nature does it).
- ReLU$=\max(0,z)$ does not saturate, although it has a vanishing gradient by definition for negative inputs.
- LeakyReLU$_\alpha = \max(\alpha z, z)$ solves this. α can be viewed as a hyperparameter (0.2, rand large leak or 0.01 for a small leak), randomised during training, or even fit for along the other parameters.
- ELU (exponential linear unit) is another choice
- Finally SELU are self-normalising ELUs. Very modern.
- GELU also trendy

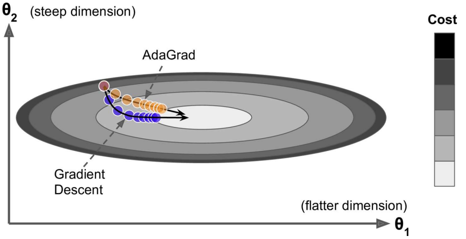
Vanishing/Exploding gradients: Batch normalisation

- Insert a normalisation step (zero centering and normalizing each input using a minibatch)
- At testing we use an exponential moving average over training for the shift parameters.
- Removes the need for standardisation if first layer is a BN layer
- Very much state-of-the-art
- Can be slower than ELU + He

Faster optimisers

- Momentum optimization
  - Give some momentum/gradient memory to the trajectory
- Nesterov Accelerate Gradient
  - Use gradients ahead of the path to nudge
- AdaGrad
  - Scales gradients along steepest directions (measured by accumulated variance in components of gradient)
  - Often stops too early due to agressive downscaling
- RMSProp
  - changes accumulation to an exponential moving average
- Adam & Nadam
  - Adaptive moment estimation
  - Combination of Momentum and RMSProp





Learning rate scheduling

- Power scheduling: $\eta(t) = \eta_0/(1+t/k)^c$
- Exponential scheduling: $\eta(t) = \eta_0 0.1^{t/s}$
- Piecewise constant scheduling
- Performance scheduling: continuous version of early stopping

Regularisation

- ℓ_1 and ℓ_2 regularisation
  - These explicitly constrain the weights, and are easy to apply e.g.

    ```
    layer = keras.layers.Dense(100, activation="elu",
                               kernel_initializer="he_normal",
                               kernel_regularizer=keras.regularizers.l2(0.01))
    ```

    (try it out! `l1` and `l1_l2` as well)
- Dropout
  - At every training step, every neuron is dropped/zeroed in the calculation with probability p
  - No dropping after training (but minor correction of $1-p$ keep probability rescaling)
  - Simple but shockingly effective
- MCDropout
  - Cambridge-based theory paper linking dropout networks with ABC [arxiv:1506.02142]
  - Puts monte-carlo dropping back into training to get errors
- Max-Norm regularisation
  - Constrain the weights so $||w||_2 < r$, clipping if needed $w \to wr/||w||_2$

DeepNet guidelines (Géron)

Hyperparameter	Default value
Kernel initializer:	LeCun initialization
Activation function:	SELU
Normalization:	None (self-normalization)
Regularization:	Early stopping
Optimizer:	Nadam
Learning rate schedule:	Performance scheduling

Don't forget to standardize the input features!

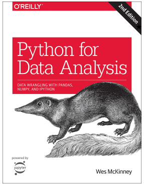
- If you need sparsity try $\ell_1\pm$ FTRL optimisation + BN
- If you need low-latency, use fewer layers, avoid BN, SELU→ReLU, consider sparsity & reducing precision
- If you are risk-sensitive consider MCDropout for performance boost and uncertainty

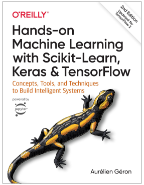
- If self-normalising & overfitting
  add α-dropout
  (do not use other regularisation)
- If cannot self normalise
  try ELU instead of SELU
  (change initialisation)
  use BN after every hidden layer
  try max-norm or ℓ_2 regularisation

Happy training!

Summary

- The data scientist's Python stack
  numpy, scipy, pandas, matplotlib, sklearn, +Keras/TensorFlow/PyTorch
- Principles & challenges of machine learning
- Theory of training, validation & testing
- Gradient descent and its pitfalls
- Regularisation and early stopping
- Neural networks Anatomy & training
- Recent advances in deep learning
  initialisation, activation, normalisation, optimisation, regularisation

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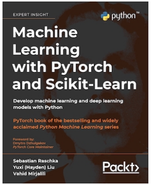
EXPERT INSIGHT
python
Machine Learning with PyTorch and Scikit-Learn
Develop machine learning and deep learning models with Python
PyTorch book of the bestselling and widely acclaimed Python Machine Learning series
Foreword by: Dmytro Dzhulgakov PyTorch Core Maintainer
Sebastian Raschka
Yuxi (Hayden) Liu
Vahid Mirjalili
Packt

What we didn't cover!

- Choosing features
- Visualisation
- Classification