

Training ML models

Cambridge ICCS summer school
cambridge-iccs.github.io/summerschool

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2022-09-22

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

- ▶ 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, $x @ y$, $z[:, \text{None}]$, ufuncs

1. scipy & pandas

- ▶ Extends numpy to numerical algorithms and excel-like array functionality
- ▶ pandas often a data scientist's weakest point

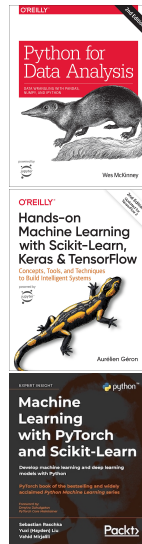
2. scikit-learn

- ▶ 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

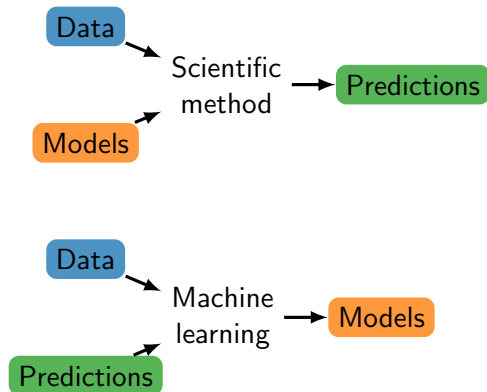
+ matplotlib for plotting (others exist, extending and reducing flexibility)



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



The machine learning pipeline

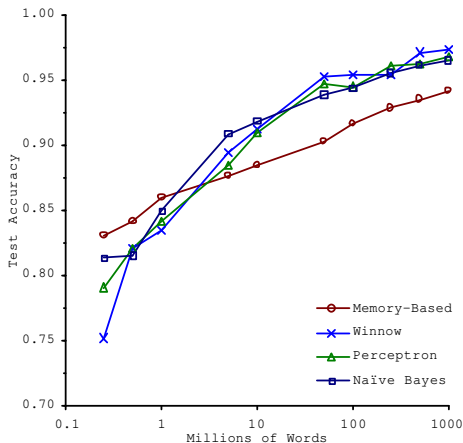
1. Problem framing
2. Data acquisition
3. Visualisation
4. Data preparation/munging
5. Selecting & training a model
6. Tuning a model
7. Launch, monitor & maintain

The machine learning pipeline

1. Problem framing
 - ▶ Big picture
 - ▶ Selecting performance measures/objectives
 - ▶ Checking assumptions/bias
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The machine learning pipeline

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

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 - ▶ Topic of this session
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The machine learning pipeline

1. Problem framing
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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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Batch

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 $\mathbf{x}^{(i)}$, output data $y^{(i)}$, where $i = 1, \dots, n_{\text{obs}}$
2. Parameterised model $y = h_{\theta}(\mathbf{x})$, where h is the model and θ are its parameters
3. Loss function(s) $L(y_{\text{pred}}, y)$

- ▶ Train the parameters on a training subset by solving the mathematical problem

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

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

$$\hat{h} = \min_h \sum_{i \in \text{validation}} L_{\text{validation}}(h_{\hat{\theta}}(\mathbf{x}^{(i)}), y^{(i)})$$

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

1. Data

- ▶ The initial data $\{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \dots, n_{\text{obs}}\}$ 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 θ , 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

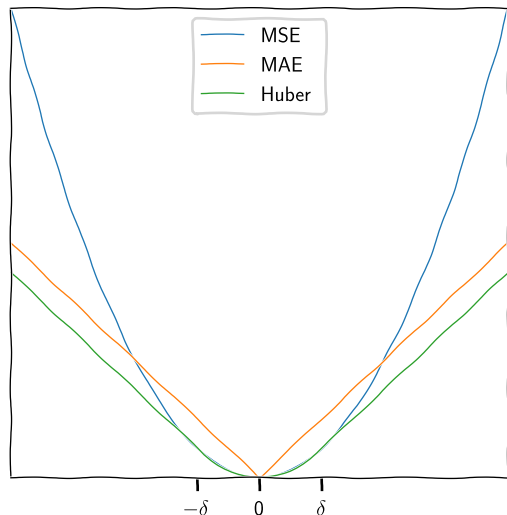
- ▶ AlphaGo
- ▶ GANs

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

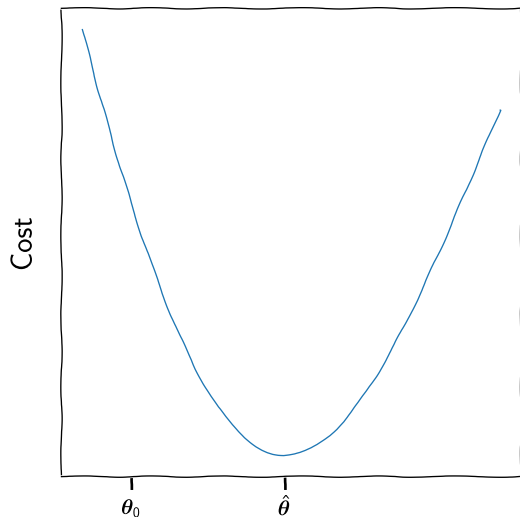
Holdout ~20% of the data.
Should be ideally “one-shot”.

- ▶ “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 $f(\theta)$, start somewhere θ_0 and go downhill (down the gradient) by some step η

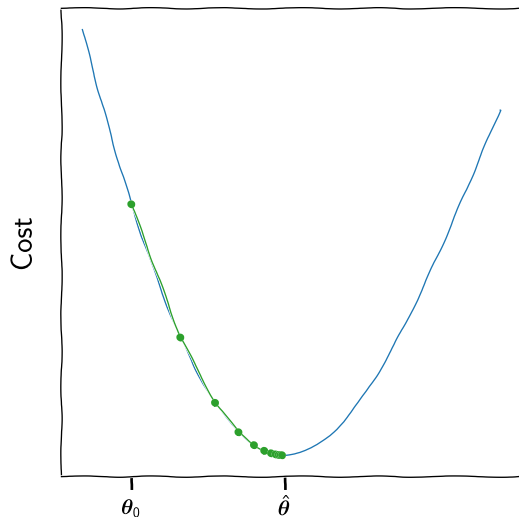
$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} f(\theta)$$



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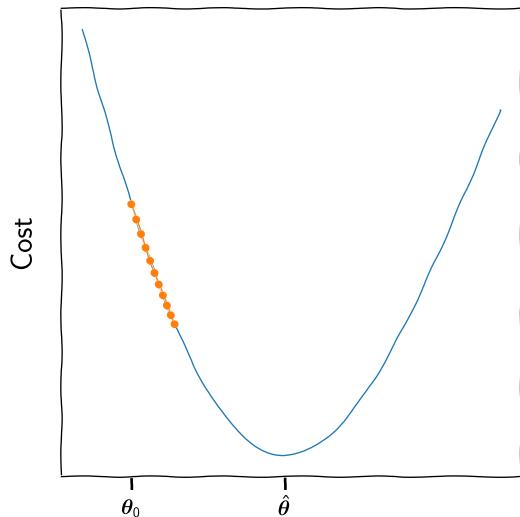


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- ▶ Problems:
 - ▶ Learning rate too slow



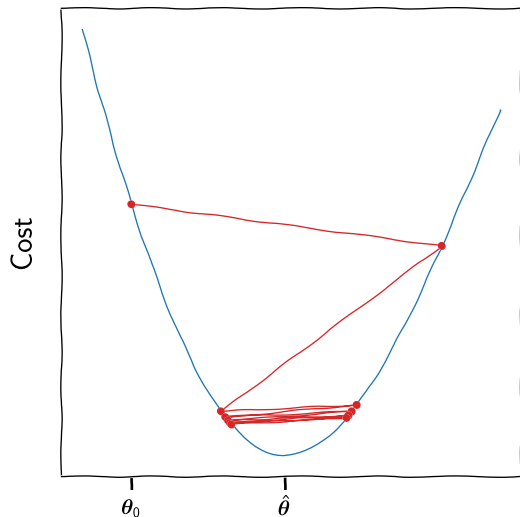
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- ▶ Problems:

- ▶ Learning rate too slow
- ▶ Learning rate too fast

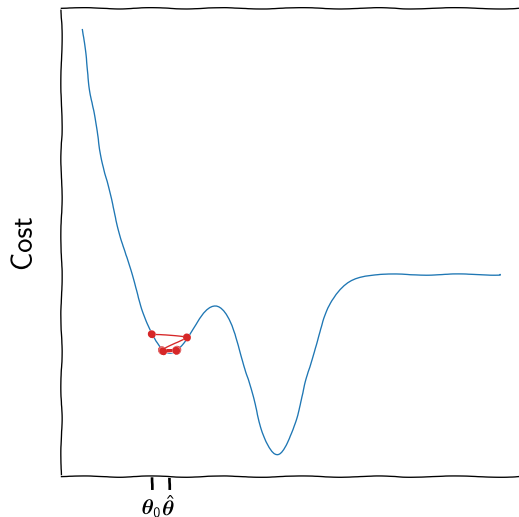


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 - ▶ Learning rate too slow
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 - ▶ Local minima



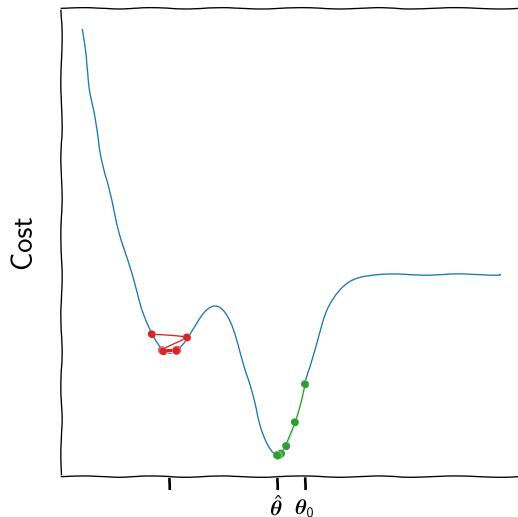
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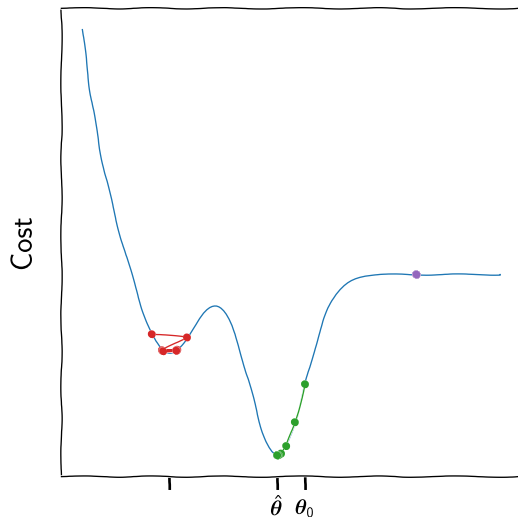
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- ▶ Local minima
- ▶ stalling



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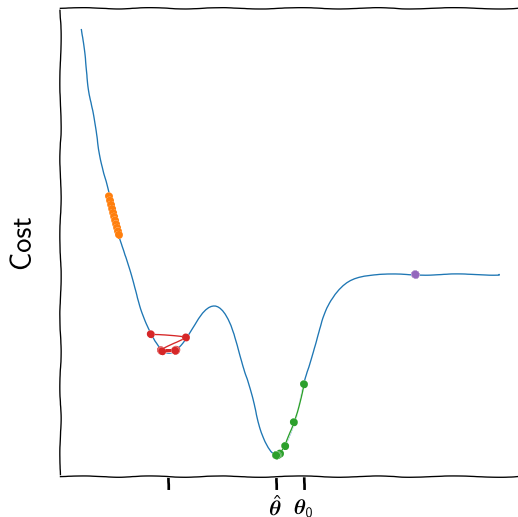
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- ▶ Problems:

- ▶ 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 $\nabla_{\theta} f(\theta)$
 1. Analytically
 - ▶ Painstakingly coding the function explicitly
 - ▶ Accurate, but practically impossible for all but the simplest functions
 2. Numerically
 - ▶ Computing finite differences $[\nabla_{\theta} f(\theta)]_i \approx [f(\theta + \delta \hat{e}_i) - f(\theta)] / \delta$
 - ▶ Easy, but prone to numerical instability
 - ▶ Expensive – costs $\sim \mathcal{O}(n)$ function evaluation for each coordinate direction \hat{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 programming 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:

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

Deterministic.

Slow for large data sets.

Stochastic gradient descent (SGD)

Compute the gradient on one random data point

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

Blazingly fast.

Randomness can escape minima.

Mini-batch gradient descent

Compute the gradient on a (small) subset of points

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

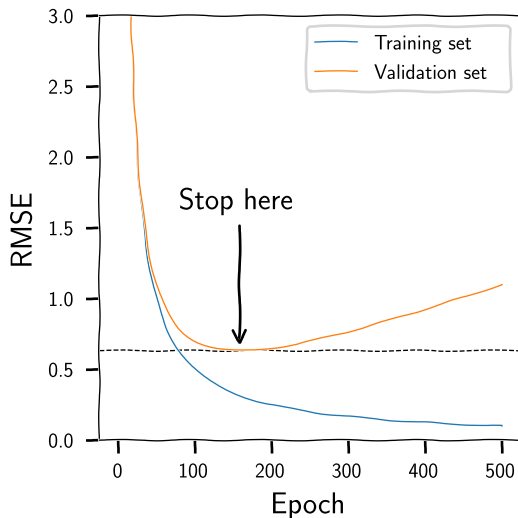
GPU accelerable.

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: $L(\theta) + \frac{1}{2}\alpha \sum_i \theta_i^2$
 - ▶ Lasso regression: $L(\theta) + \alpha \sum_i |\theta_i|$
 - ▶ Least absolute shrinkage & selection operator
 - ▶ Promotes sparsity
 - ▶ Elastic Net: $L(\theta) + r\alpha \sum_i |\theta_i| + \frac{1-r}{2}\alpha \sum_i \theta_i^2$
- ▶ 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

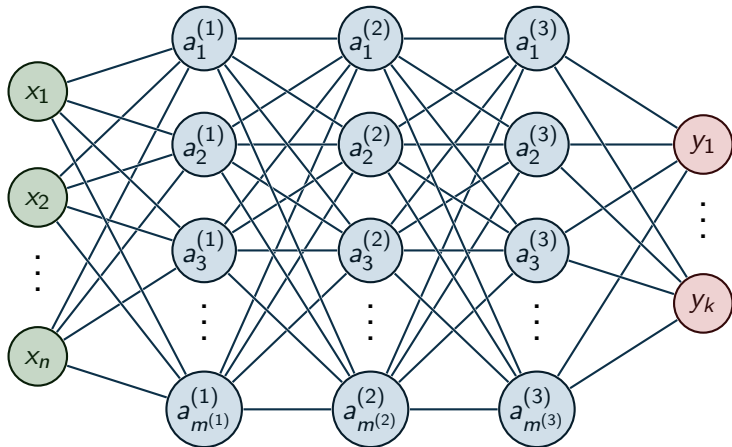
$$a_i^{(\ell+1)} = \phi_i^{(\ell)} \left(\sum_{j=1}^{m^{(\ell)}} w_{ij}^{(\ell)} a_j^{(\ell)} + b_i^{(\ell)} \right)$$

or written in vectors:

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

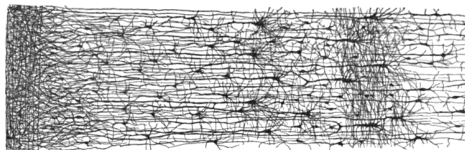
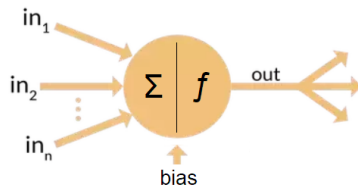
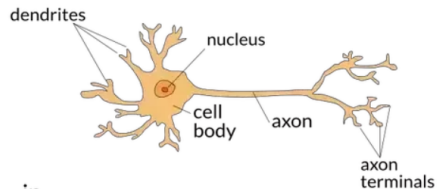
$$\mathbf{a}^{(0)} = \mathbf{x}, \quad \mathbf{y} = \mathbf{a}^{(m+1)}$$

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 $\mathbb{R}^n \rightarrow \mathbb{R}^k$ 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

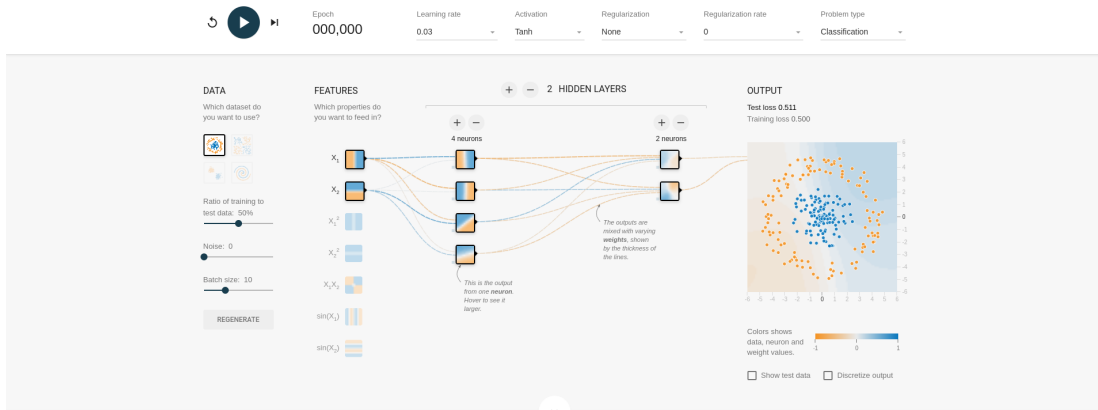
Anatomy

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

Training

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

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

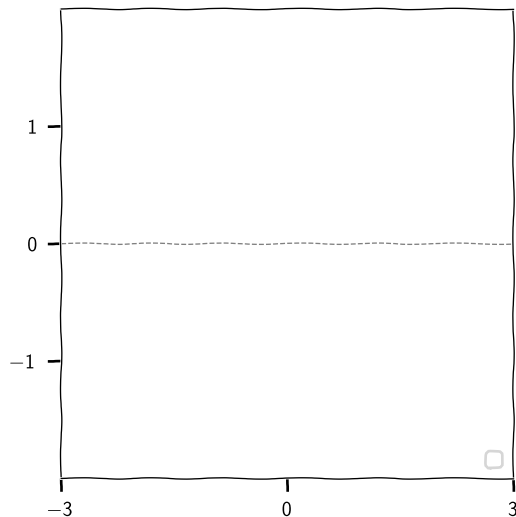


Hyperparameter tuning

- ▶ 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

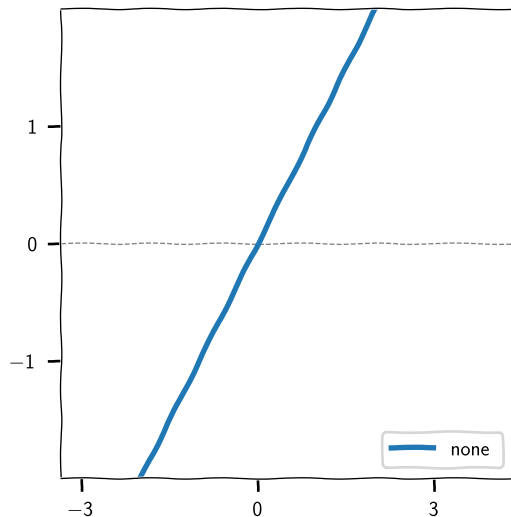
Activation functions

- ▶ 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



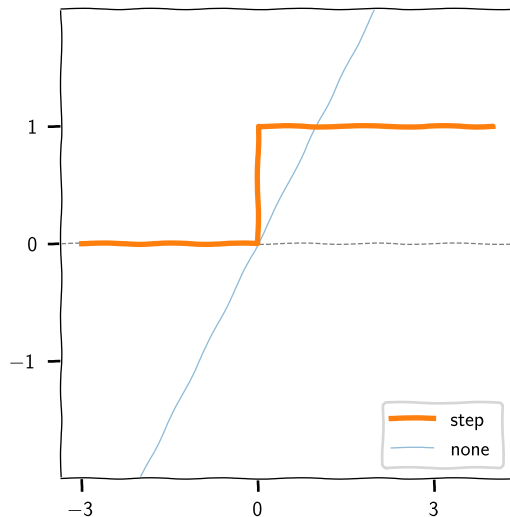
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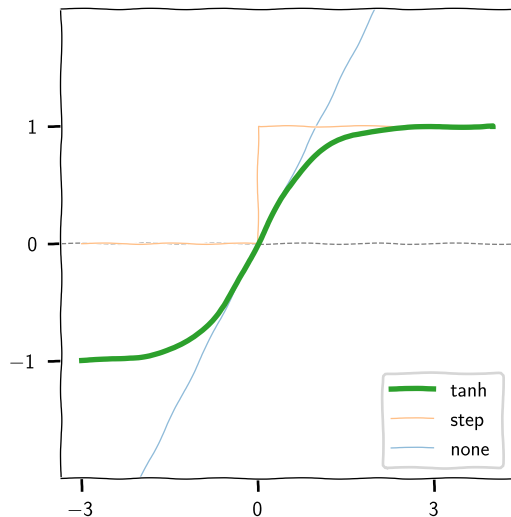
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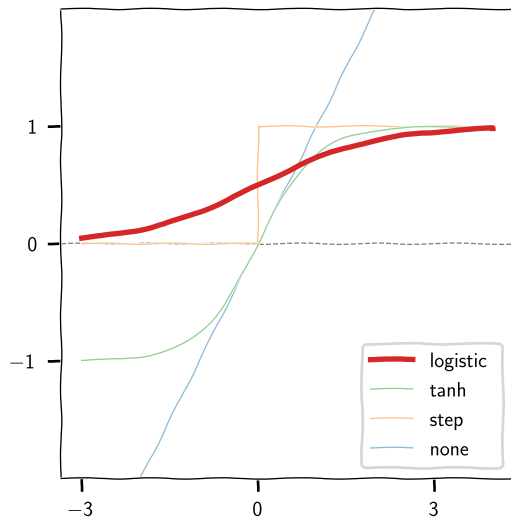
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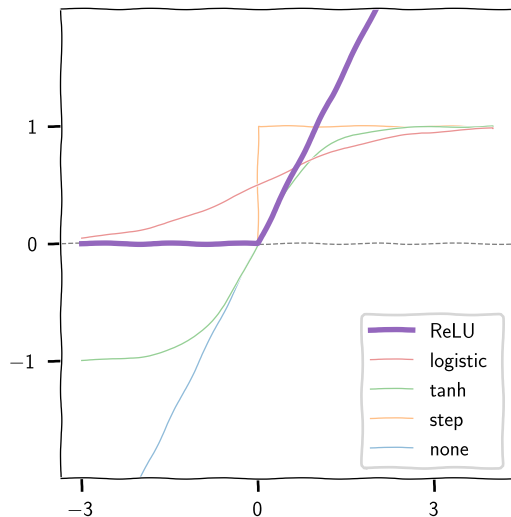
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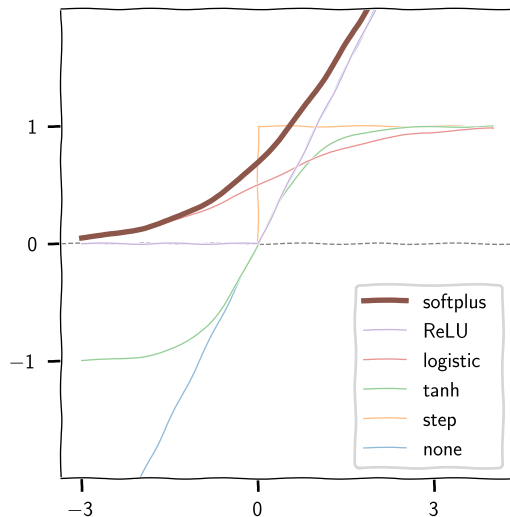
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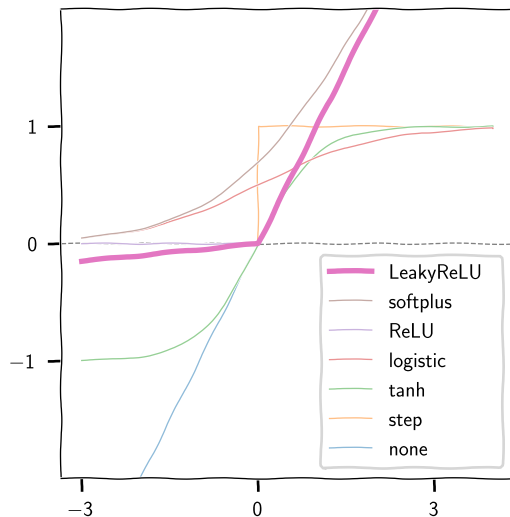
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 - ▶ For inner layers one may want symmetry/infinite range



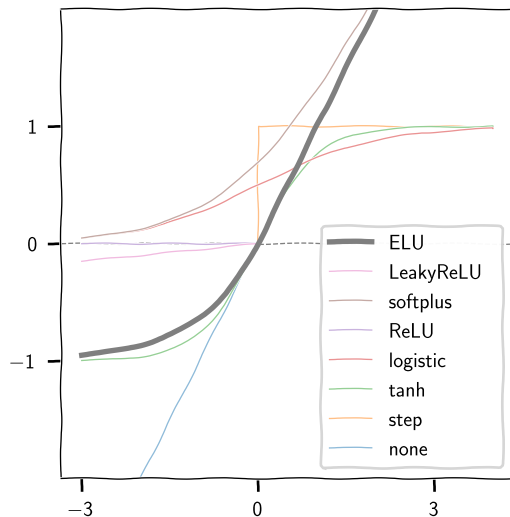
Activation functions

- ▶ There is now a veritable zoo of activation functions
- ▶ Important properties to consider:
 - ▶ Smoothness
 - ▶ Saturation (at either end)
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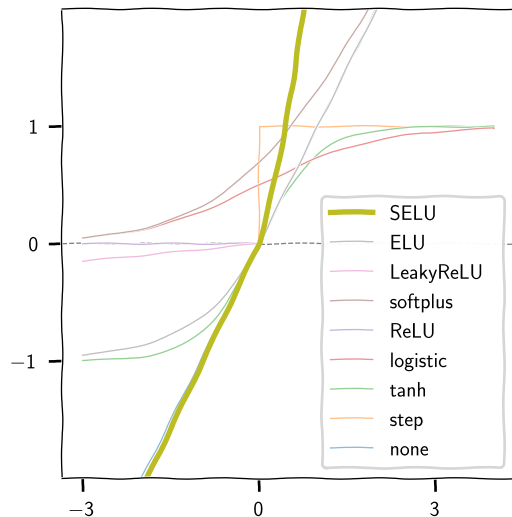
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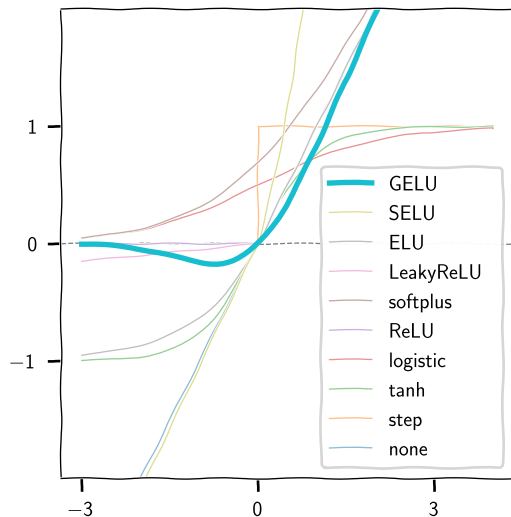
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Typical architectures

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 too 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 (θ_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: $\text{fan}_{\text{avg}} = \frac{1}{2}(\text{fan}_{\text{in}} + \text{fan}_{\text{out}})$, where $\text{fan}_{\text{in}} \equiv$ circuit terminology to describe the number of inputs to a layer

Glorot

Activation: None, Tanh, logistic, softmax.

initialise weights: Normal with variance

$$\sigma^2 = \frac{1}{\text{fan}_{\text{avg}}} \text{ (or Uniform in } \pm\sqrt{3/\text{fan}_{\text{avg}}}\text{)}$$

He

Activation: ReLU *et al.*

initialise weights:

$$\text{variance } \sigma^2 = \frac{2}{\text{fan}_{\text{in}}}$$

Lecun

Activation: SELU

initialise weights:

$$\text{variance } \sigma^2 = \frac{1}{\text{fan}_{\text{in}}}$$

Vanishing/Exploding gradients: Nonsaturating activation functions

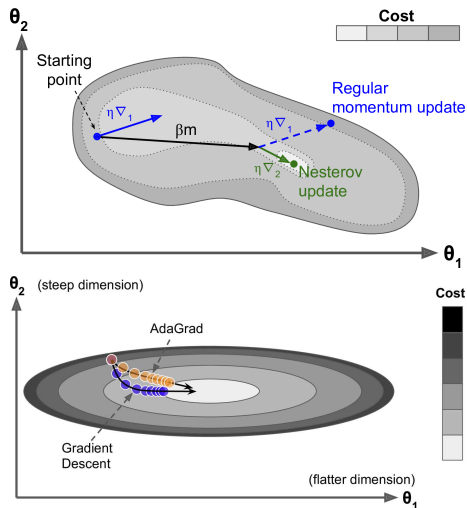
- ▶ Another way to fix the saturation problem is to choose a nonsaturating activation function (N.B. This is not how mother nature does it).
- ▶ $\text{ReLU} = \max(0, z)$ does not saturate, although it has a vanishing gradient by definition for negative inputs.
- ▶ $\text{LeakyReLU}_\alpha = \max(\alpha z, z)$ 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 aggressive 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! ℓ_1 and $\ell_{1,2}$ 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 $w \rightarrow wr/\|w\|_2$

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!

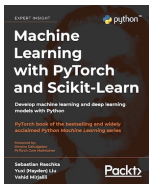
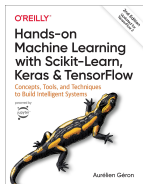
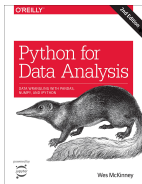
- ▶ If you need sparsity try $\ell_1 \pm$ FTRL optimisation + BN
- ▶ If you need low-latency, use fewer layers, avoid BN, SELU \rightarrow ReLU, consider sparsity & reducing precision
- ▶ If you are risk-sensitive consider MCDropout for performance boost and uncertainty

- ▶ 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



What we didn't cover!

- ▶ Choosing features
- ▶ Visualisation
- ▶ Classification