Neural Networks

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Outline

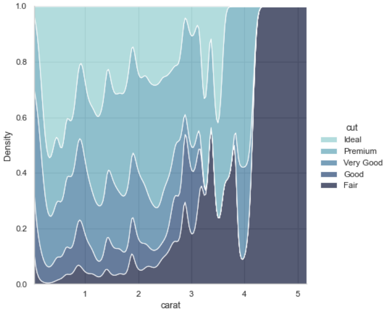
- Modelling nonlinearities
- Neural Network
- Training
- Going deeper
- Tackling overfitting
- NN zoo

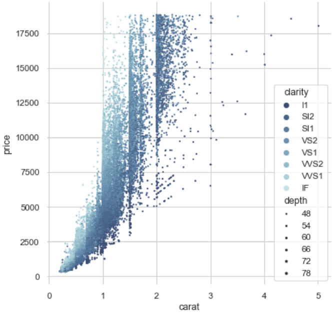
Modelling nonlinearities

Modelling nonlinearities

they exist

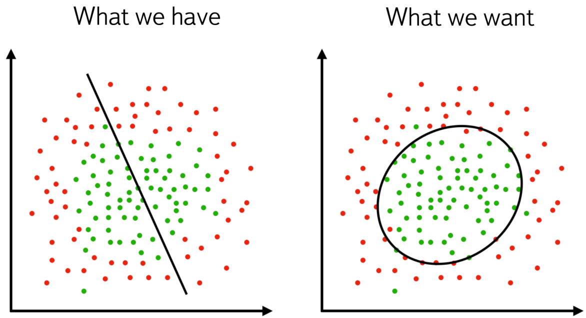
seaborn illustrations





Modelling nonlinearities

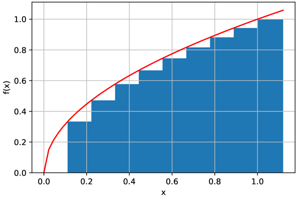
linear models

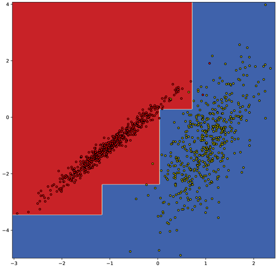


Linear models can't simply describe complex nonlinear data

Modelling nonlinearities

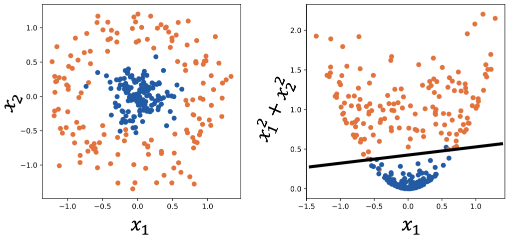
trees





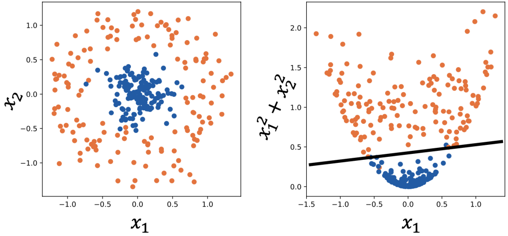
- (Ensembles of) Trees were designed to approximate nonlinearities and are **pretty good** in it + they are **fast and interpretable**
- But they are just "brute-force" algorithms – **don't infer symmetries** in data by design
- **Ad-hoc, cut-based and piecewise approximations** of data at hand + not differentiable and smooth

Modelling nonlinearities — feature engineering



- But sometimes we know *a priori* that there are transformations simplifying the problem $\rightarrow$ even linear model can do the job
- However, this **feature engineering** is non-trivial, requires domain knowledge and is time-consuming

Modelling nonlinearities — feature engineering



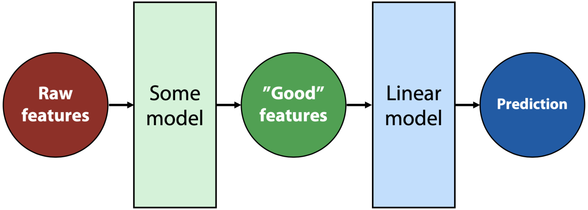
- But sometimes we know *a priori* that there are transformations simplifying the problem $\rightarrow$ even linear model can do the job
- However, this **feature engineering** is non-trivial, requires domain knowledge and is time-consuming

What if we design a model which could **automatically** feature-engineer itself?

Neural Network

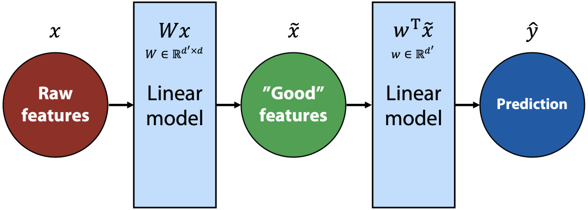
Neural Network → automating FE

NN illustrations from
ML in HEP 2020



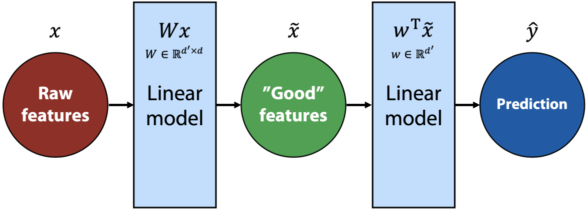
- Let's use a **simple linear model** to solve our supervised problem
- Add a block to a linear model which will automatically **generate new features** for it
- Two blocks would work together as a **single model** $\Rightarrow$ their parameters are updated simultaneously
- And **automatically**, by e.g. gradient descent (given their differentiability)

Neural Network — automating FE



- Would a linear model work as a feature generating model?

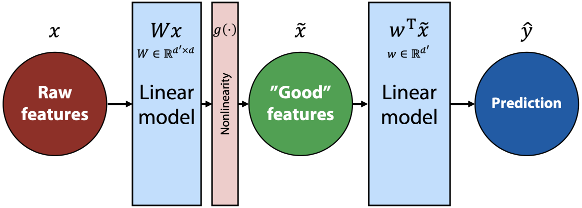
Neural Network — automating FE



- Would a linear model work as a feature generating model? No
- $\hat{y} = w^T \tilde{x} = w^T (Wx) = (w^T W)x = w'^T x \Rightarrow$ it is still a linear model

➔ Input feature space has not changed, only the model weights

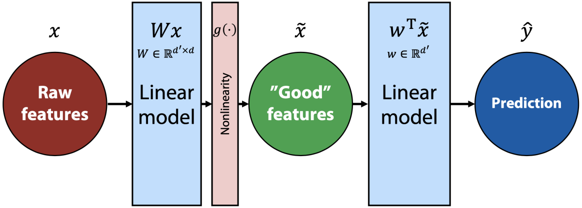
Neural Network — automating FE



- Let's then introduce **nonlinearity** to our model

→ $\hat{y} = w^T \tilde{x} = w^T g(Wx)$,
where $g(\cdot)$ – some nonlinear scalar function (applied elementwise)

Neural Network — automating FE



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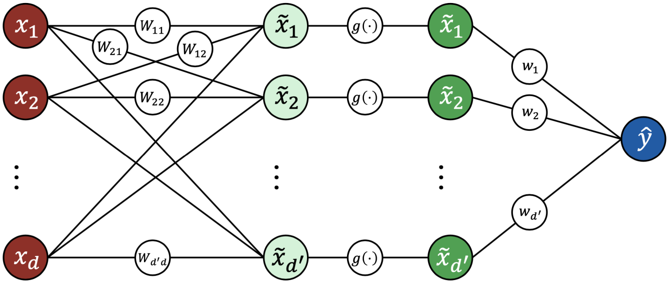
→ $\hat{y} = w^T \tilde{x} = w^T g(Wx)$,
where $g(\cdot)$ – some nonlinear scalar function (applied elementwise)

→ This is the simplest example of a **neural network**

Neural Network — architecture

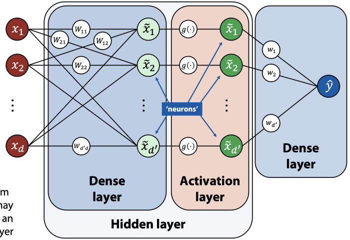


Essentially, NN is just a **composite function** that maps a set of X to a set of Y

$$\hat{y} = w^T \tilde{x} = w^T g(Wx)$$

Neural Network — terminology

Feed-forward network:

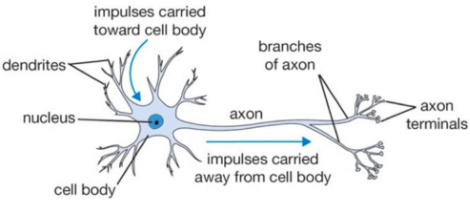


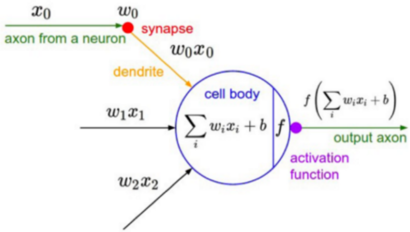
Note: the term "activation" may also stand for an output of a layer

- Brown nodes $x_1, x_2, ..., x_d$ – features from an **input layer**
- Green nodes $\tilde{x}_1, \tilde{x}_2, ..., \tilde{x}_{d\prime}$– **neurons** from a **hidden layer**
- Blue node $\hat{y}$ – neuron from an **output layer**
- Straight lines (edges) between neurons – **weights** w_{ij}
- $g(\cdot)$ – nonlinear **activation** function, e.g. sigmoid $\sigma(\cdot)$
- Important: each neuron has additional **bias** b associated to it and added to other inputs (not illustrated)

Neural Network

human brain





Training

Training — how to train?

- Since NN fundamentally is a parametrized differentiable model we can optimise the loss function and use **gradient descent** to train it:

$$\omega_{k+1} \leftarrow \omega_k - \eta \cdot \nabla Q(\omega_k)$$

- But gradients are hard to derive analytically – writing down all the derivatives is tough and tedious (especially for large NN)
- Note that NN is just a **composite model** $\Rightarrow$ can use **chain rule** for differentiating it

Training — chain rule

- Computing derivative of a ”base” function is simple $\Rightarrow$ decompose composite function into a set of base ones and differentiate them one by one
- Let's recall the rule:

$$\frac{\partial f\big(t(x)\big)}{\partial x} = \frac{\partial f(t)}{\partial t} \cdot \frac{\partial t(x)}{\partial x}$$

Exercise: can you compute derivative of sigmoid function by decomposing it into base functions?

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$\sigma(x) = f(g(h(p(x)))), \quad f(z) = \frac{1}{z}, \quad g(z) = 1 + z, \quad h(z) = e^z, \quad p(z) = -z$$

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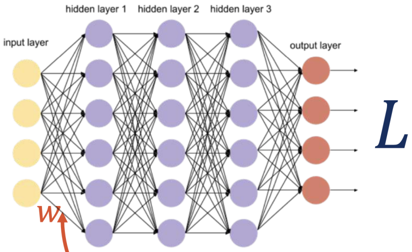
$$\sigma'(x) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial p} \cdot \frac{\partial p}{\partial x} = -\frac{1}{g^2} \cdot 1 \cdot e^p \cdot (-1) = \ldots = \sigma(x) \cdot \big(1-\sigma(x)\big)$$

Training — backpropagation

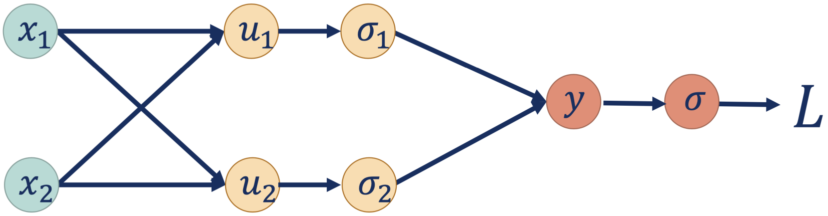
backprop illustrations from DMIA



$$w^{(t+1)} = w^{(t)} - \gamma_t \boxed{\frac{\partial L}{\partial w}}$$

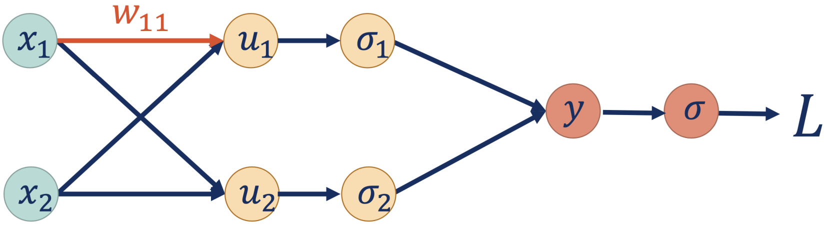
- So how to find partial derivatives of loss function with respect to some weight?

backprop illustrations from DMIA



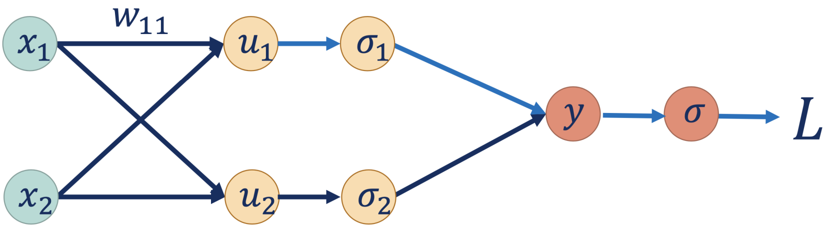
- Let's consider a simplified neural network
- Represent it in the form of a **computational graph**

Training — backpropagation



$$w_{11}^{(t+1)} = w_{11}^{(t)} - \gamma_t \frac{\partial L}{\partial w_{11}}$$

Training — backpropagation

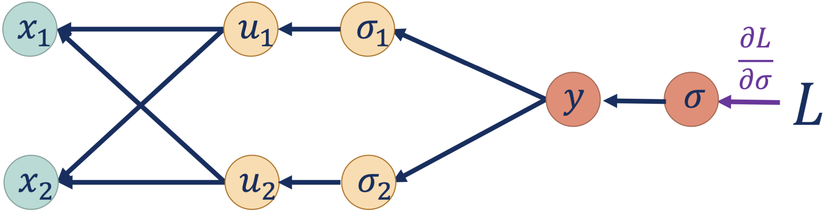


$$w_{11}^{(t+1)} = w_{11}^{(t)} - \gamma_t \frac{\partial L}{\partial w_{11}}$$

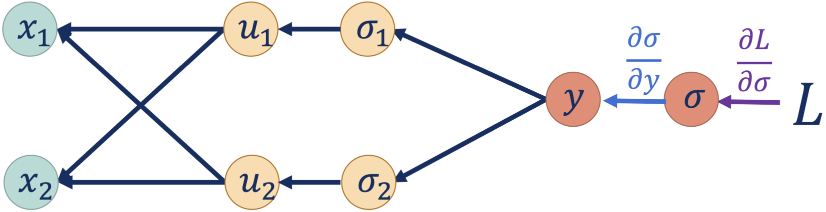
$$\boxed{\frac{\partial L}{\partial w_{11}} = \frac{\partial L}{\partial u_1}\frac{\partial u_1}{\partial w_{11}} = \frac{\partial L}{\partial u_1} x_1}$$

Training

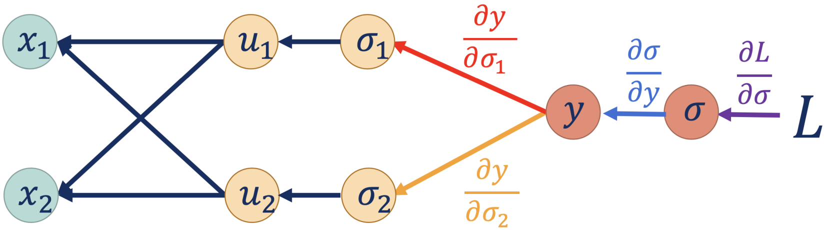
backpropagation



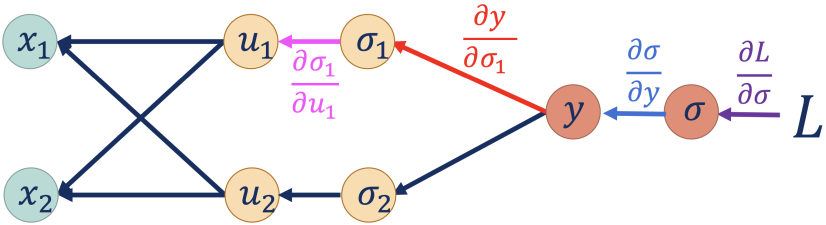
Training — backpropagation



Training — backpropagation

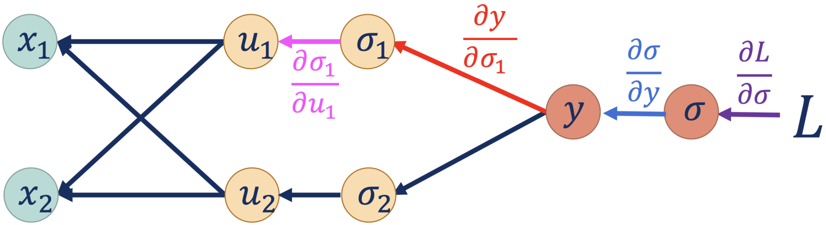


Training —o backpropagation



$$\frac{\partial L}{\partial u_1} = \frac{\partial L}{\partial \sigma}\frac{\partial \sigma}{\partial y}\frac{\partial y}{\partial \sigma_1}\frac{\partial \sigma_1}{\partial u_1}$$

Training — backpropagation

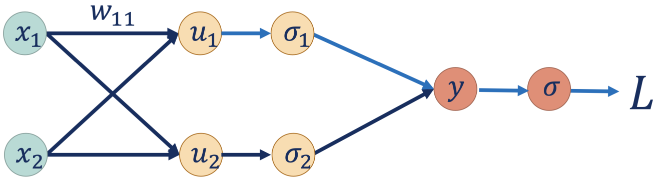


$$\frac{\partial L}{\partial u_1} = \frac{\partial L}{\partial \sigma}\frac{\partial \sigma}{\partial y}\frac{\partial y}{\partial \sigma_1}\frac{\partial \sigma_1}{\partial u_1}$$

- this procedure is called **backpropagation**
- its idea is to **collect derivatives** at each step in the computational graph w/o recalculating them every single time for every weight

Training — wrap it up

train NN in your browser!



1. make **forward pass** through NN to calculate the output of each neuron and value of loss function

Training — wrap it up

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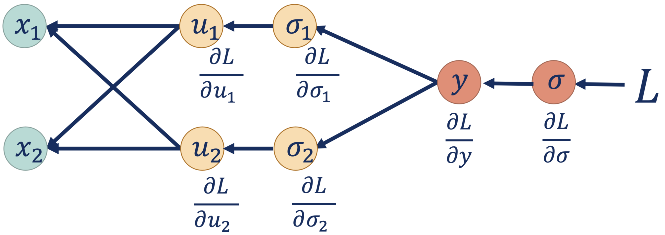

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2. with **backward pass** go back through NN to calculate gradients for all weights

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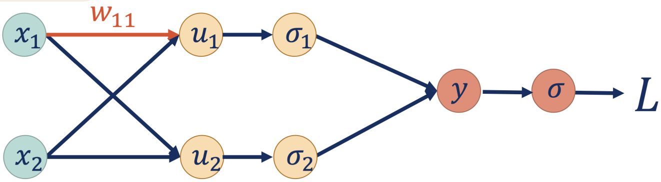

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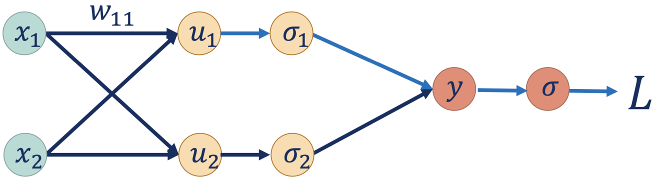


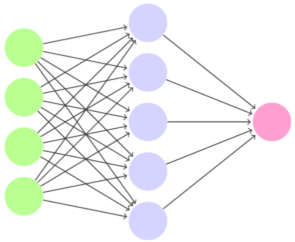
1. make **forward pass** through NN to calculate the output of each neuron and value of loss function
2. with **backward pass** go back through NN to calculate gradients for all weights
3. update weights with their gradients
4. repeat until convergence

*one iteration (**epoch**) = forward and backward pass

Going deeper

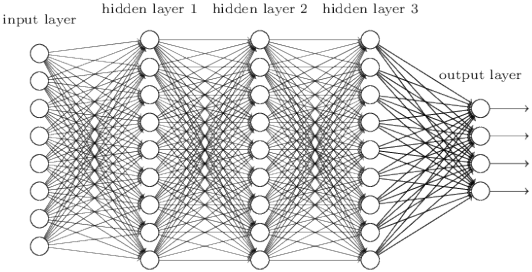
Going deeper — universal approximation theorem

- Roughly speaking, any well-behaved function f can be approximated **arbitrarily close** with a 1-hidden layer NN, given wide enough hidden layer
- But in practice this is often not the case:
  - loss function is heavily non-convex
  - overfitting
  - not straightforward how to find this NN



Going deeper — stack more layers

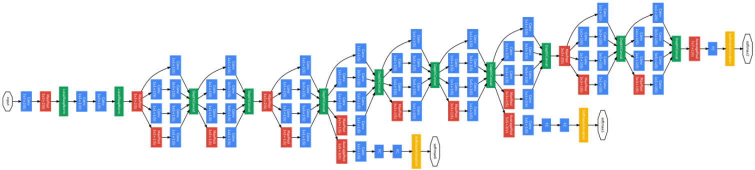
- In practice stacking more layers generally **improves performance**

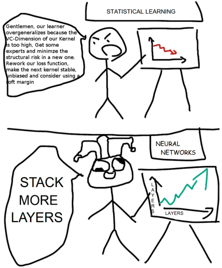


Going deeper — stack more layers

Going deeper with convolutions

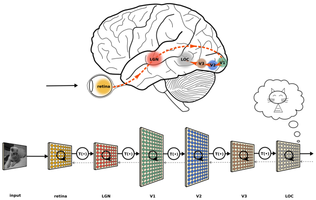
- In practice stacking more layers generally **improves performance**
- Much more layers...





Going deeper

- In practice stacking more layers generally **improves performance**
- Much more layers...
- Which is reminiscent of the **brain structure**
- Signals travel through multiple areas of different organization
- This makes our perception system incredibly advanced in understanding reality



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→ but there are some problems...

Going deeper — vanishing gradients

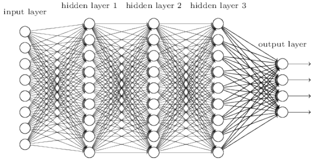
- Layer $f_i(\boldsymbol{z_{i-1}})$ takes the output $\boldsymbol{z_{i-1}}$ from the previous layer and returns $\boldsymbol{z_i}$
- Using chain rule and sigmoid activation we have:

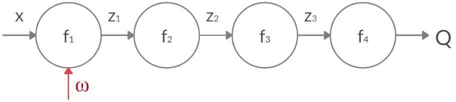
$$\Delta\omega_j \sim \frac{\partial Q}{\partial \omega_j} = \frac{\partial Q}{\partial f_i}\frac{\partial f_i}{\partial f_{i-1}}\cdots\frac{\partial f_1}{\partial \omega_j}$$

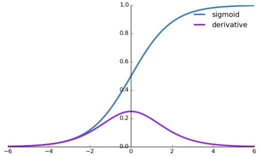
$$\frac{\partial f_i}{\partial f_{i-1}} = \sigma(z_{i-1})\big(1-\sigma(z_{i-1})\big)$$

- $$\left|\frac{\partial f_i}{\partial f_{i-1}}\right| \leq \frac{1}{4} \Rightarrow \frac{\partial Q}{\partial \omega_j} \lesssim \left(\frac{1}{4}\right)^n \Rightarrow \boldsymbol{\Delta\omega_j \to 0,\ n \to \infty}$$

➔ there's no learning happening







- Let's have a closer look at sigmoid activation:

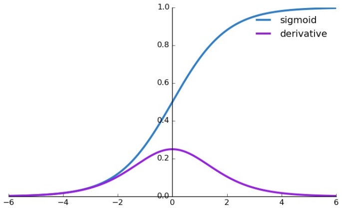
$$\sigma(z) = \frac{1}{1+e^{-z}}$$

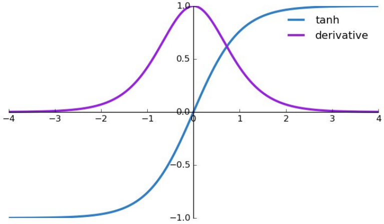
→ outputs are in [0,1] range ⇒ "neuron fired" intuition

→ outputs are not zero-centered

→ **saturate at large** $|z|$ ⇒ **kill gradients** ($\to 0$)

- same applies to $\tanh(z) = \dfrac{e^z - e^{-z}}{e^z + e^{-z}}$





Going deeper → activation functions

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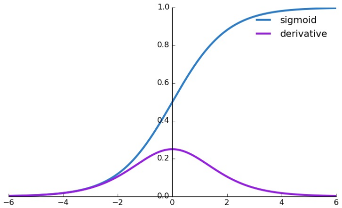
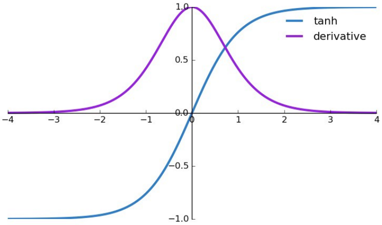
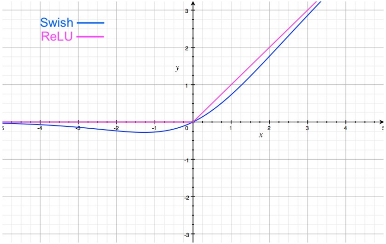
→ can we use other activation functions?





- ReLU(x) $= \max(0, z)$
  - → gradients don't vanish
  - → simple implementation (derivative either 0 or 1)
  - → not zero-centered and unbounded
  - → neurons can "die"
  - → there's more: Leaky ReLU, ELU, GELU, Softplus
- and even more:

e.g., Swish(z) $= \dfrac{z}{1 + e^{-\beta \cdot z}} = z \cdot \sigma(\beta \cdot z)$



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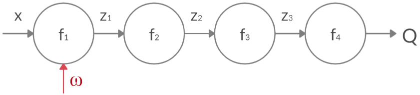
- Intuitively, weights are updated by:

$$\Delta\omega_j \sim \frac{\partial Q}{\partial f_i}\frac{\partial f_i}{\partial f_{i-1}}\cdots\frac{\partial f_1}{\partial \omega_j} \sim \prod_i S_{ij}$$

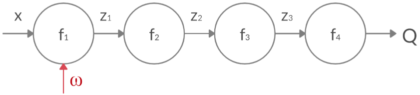
S_{ij} - scale of gradient at i-th layer



- if $S_{ij} \ll 1$, gradients vanish and weights don't update $\Rightarrow$ learning is stuck
- if $S_{ij} \gg 1$, gradients explode $\Rightarrow$ learning is extremely unstable

init playground

- But gradients can also **explode**
- Intuitively, weights are updated by:



$$\Delta\omega_j \sim \frac{\partial Q}{\partial f_i}\frac{\partial f_i}{\partial f_{i-1}}\cdots\frac{\partial f_1}{\partial \omega_j} \sim \prod_i S_{ij}$$

S_{ij} - scale of gradient at i-th layer

- if $S_{ij} \ll 1$, gradients vanish and weights don't update $\Rightarrow$ learning is stuck
- if $S_{ij} \gg 1$, gradients explode $\Rightarrow$ learning is extremely unstable

Idea: constrain the scales at each layer to avoid exponential growth

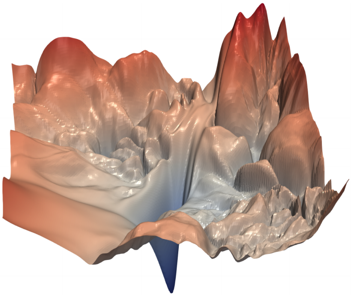
→ one can show that clever weight initialisation can remedy this

→ e.g. Xavier: $W_j \sim \mathcal{N}\left(0, \frac{1}{n_{\text{in}}}\right)$ or He: $W_j \sim \mathcal{N}\left(0, \frac{2}{n_{\text{in}}}\right)$ (for ReLU) initialisations*

*library implementations may slightly differ

Tackling overfitting

- NN are higly complicated models with $>$ 1M weights being normal
- Therefore, optimisation task is extremely tough with loss function being non-convex
- This makes overfitting and getting trapped in a local minimum a piece of cake



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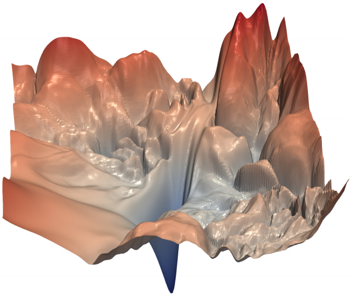
→ Improvements in optimisation methods are needed



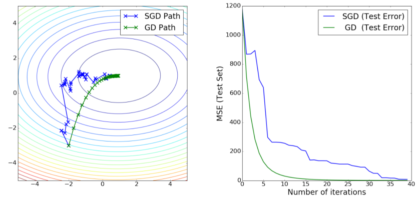
- **SGD:**
  - At each step k pick random sample $(\boldsymbol{x}_l, y_l)$
  - Update weights:

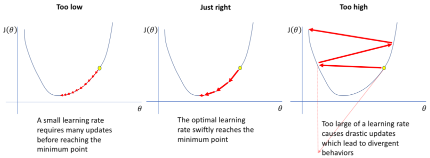
$$\boldsymbol{\omega}^{(k)} \leftarrow \boldsymbol{\omega}^{(k-1)} - \eta \nabla Q\left(y_l, f_{\omega}(\boldsymbol{x}_l)\right)\Big|_{\boldsymbol{\omega}=\boldsymbol{\omega}^{(k-1)}}$$

- **Mini-batch SGD:**
  - Iterate through the dataset in chunks (batches)
  - Aggregate gradients over the chunk:

$$\boldsymbol{g} = \sum_{l \in B} \nabla Q\left(y_l, f_{\omega}(\boldsymbol{x}_l)\right)$$

  - Update the weigths: $\boldsymbol{\omega}^{(k)} \leftarrow \boldsymbol{\omega}^{(k-1)} - \eta \cdot \boldsymbol{g}$



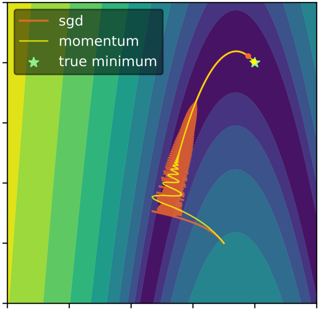


check out more on distill

- Let's change perspective to a physical one and add a notion of **velocity**
- Example: a ball rolling down the hill $\Rightarrow$ treat loss as **potential energy**
- If we build up velocity in a direction with consistent gradient, we can overcome local minima and smooth out rapid oscillations $\Rightarrow$ **SGD with momentum**:

$$\boldsymbol{v}^{(k)} \leftarrow \beta \boldsymbol{v}^{(k-1)} - \eta \nabla Q\left(y_l, f_\omega(\boldsymbol{x}_l)\right)\Big|_{\boldsymbol{\omega}=\boldsymbol{\omega}^{(k-1)}}$$

$$\boldsymbol{\omega}^{(k)} \leftarrow \boldsymbol{\omega}^{(k-1)} + \boldsymbol{v}^{(k)}$$



source

Tackling overfitting — momentum

check out more on distill

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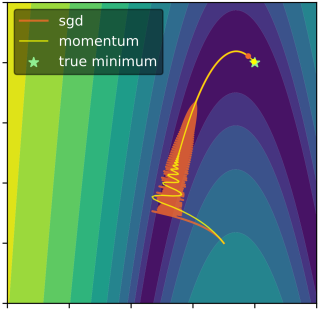
- **Nesterov momentum** updates position with "lookahead" gradient $\nabla Q\left(y_l, f_\omega(\boldsymbol{x}_l)\right)\Big|_{\boldsymbol{\omega}=\boldsymbol{\omega}^{(k-1)}+\beta\boldsymbol{v}^{(k-1)}}$



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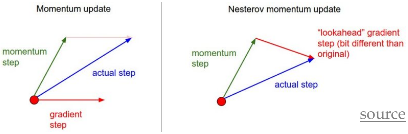

source

- Previously, we were manipulating learning rate η **globally and equally** for all parameters
- This sounds like a limitation, since gradient scales vary significanty and we could've gained from adjusting LRs for **each component independently**

Tackling overfitting — adaptive LR

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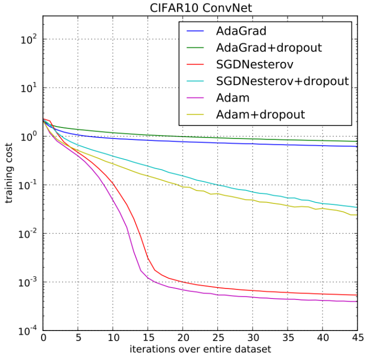
- So here comes RMSprop (Hinton's lecture notes):

$$\mathbf{Var}[g^2]_{(k)} \leftarrow \beta \cdot \mathbf{Var}[g^2]_{(k-1)} + (1-\beta)\left(\frac{\partial Q}{\partial \boldsymbol{\omega}}\right)^2 \Bigg|_{\boldsymbol{\omega}=\boldsymbol{\omega}^{(k-1)}}$$

$$\boldsymbol{\omega}^{(k)} \leftarrow \boldsymbol{\omega}^{(k-1)} - \frac{\eta}{\sqrt{\mathbf{Var}[g^2]_{(k)} + \varepsilon}} \frac{\partial Q}{\partial \boldsymbol{\omega}} \Bigg|_{\boldsymbol{\omega}=\boldsymbol{\omega}^{(k-1)}}$$

- Adam combines ideas of momentum and RMSprop

  Note: there's also LR annealing and more sophisticated optimizers



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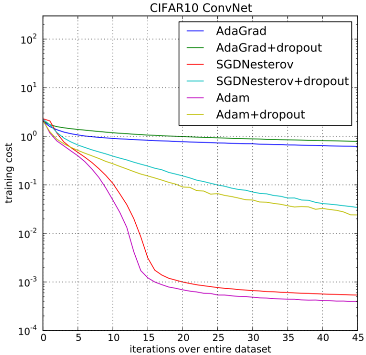
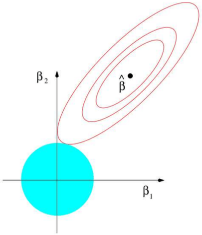


Nice moment to show this animation

Tackling overfitting — weight regularisation

L2 regularization (Tikhonov)

$$Q(\omega) = \mathbb{E}_{p(x,y)}\left[\mathcal{L}(y, f(x,\omega))\right] + \lambda \sum_{j=1}^{K} \omega_j^2$$

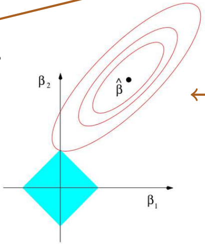


penalize model for too large weights

L1 regularization (LASSO)

least absolute shrinkage and selection operator

$$Q(\omega) = \mathbb{E}_{p(x,y)}\left[\mathcal{L}(y, f(x,\omega))\right] + \lambda \sum_{j=1}^{K} |\omega_j|$$

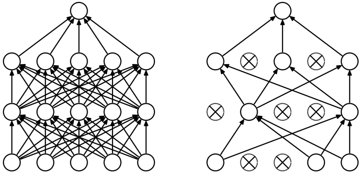


autozeroing uninformative weights!

Tackling overfitting — dropout

paper

- Let's randomly **drop neurons with probability** p during the training
- Essentially, this would mean that at each iteration we train a *new subnetwork*
- This allows for **breaking co-adaptation** of neurons $\Rightarrow$ neurons forced to learn useful features w/o relying on neighbouring ones
- And makes it very simple, elegant and **powerful regularization** technique



(a) Standard Neural Net (b) After applying dropout.

Tackling overfitting — dropout

paper

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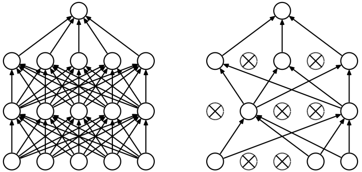
  Note: during testing one needs to simply scale neurons' outputs with p to compensate *on average* for dropout during the training



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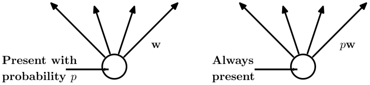
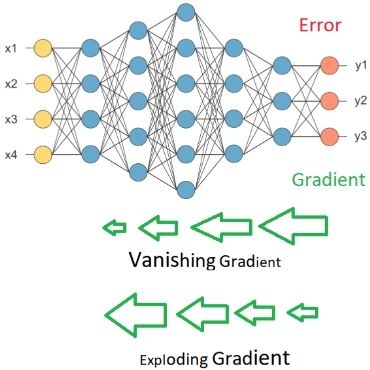


(a) At training time (b) At test time

Tackling overfitting → batch normalisation

paper

- As was mentioned earlier, training procedure is sensitive to the scale of gradients in NN
- Furthermore, the latter is connected to the inputs' scale of layers, which in turn tends to vary throughout the training (aka **"internal covariate shift"**)
- This slows down the training and makes the procedure sensitive to weight initialisation



Tackling overfitting — batch normalisation

paper

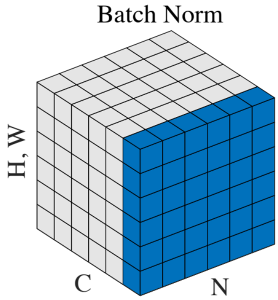
- It was proposed to approach this problem with **normalising layer inputs** over a batch (γ and β are learnable parameters):

$$\mu_B = \frac{1}{|B|}\sum_{i\in B} x_i, \qquad \sigma_B^2 = \frac{1}{|B|}\sum_{i\in B}(x_i - \mu_B)^2$$

$$y_i = \gamma \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} + \beta$$

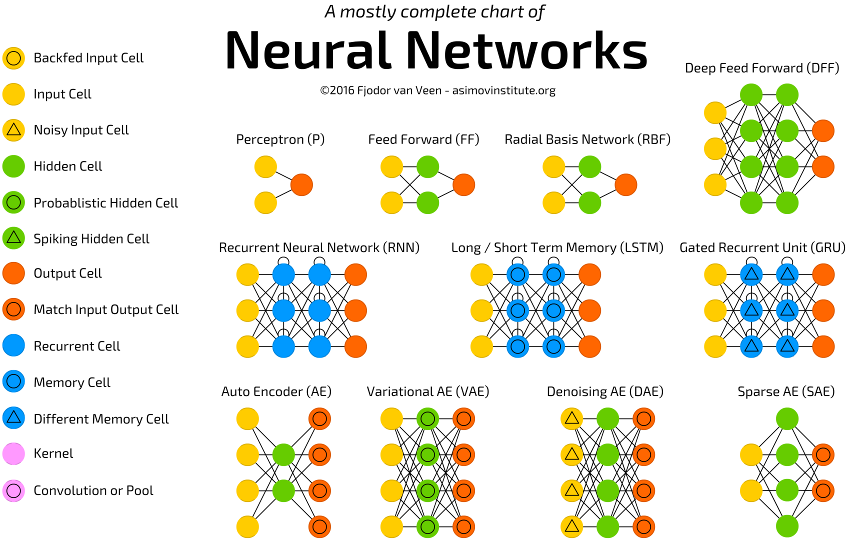
- This turned out to improve performance, speed up and stabilize convergence (but didn't really remove internal covariate shift)

Note: there are other fancy ways to normalize inputs



NN zoo

link


A mostly complete chart of
Neural Networks
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Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)

Summary

- Modelling nonlinearities
- Neural Network
  - automating feature engineering
  - architecture
  - terminology
- Training
  - chain rule
  - backpropogation
- Going deeper
  - universal approximation theorem
  - vanishing gradients
  - activation functions
  - weight initialisation
- Tackling overfitting
  - gradient descent modifications
  - weight regularization
  - dropout
  - batch normalisation
- NN zoo