Machine Learning

Neural Networks and Deep Learning: Regularization & Optimization

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Regularization

Regularization

- Central problem in ML: how to make an algorithm perform well not just on training data, but also on new inputs?
- Regularization: strategies explicitly designed to reduce the test error (i.e., improve generalization), possibly at the expense of increased training error
- Many forms of regularization
    - e.g., extra constraints on the model (possibly coming from prior knowledge, or just to express generic preference for simpler model classes)
    - e.g., additional terms in the objective function
    - e.g., ensemble methods
- We aim to trade increased bias for reduced variance

Parameter Norm Penalties

- Common regularization approach: adding a penalty $\Omega(\boldsymbol{\theta})$ to the objective function J

$$\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) + \lambda\Omega(\boldsymbol{\theta}) \quad (1)$$

where $\lambda \in (0, \infty)$ is a hyperparameter that weighs the relative importance of the penalty term.

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  where $\lambda \in (0, \infty)$ is a hyperparameter that weighs the relative importance of the penalty term.
- Usually, only applied to the connection weights (i.e., $\Omega(\boldsymbol{\theta}) = \Omega(\boldsymbol{w})$), where $\boldsymbol{w}$ indicates all the weights
  - Regularizing biases doesn't give much generalization benefit and can lead to significant underfitting

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- Usually, only applied to the connection weights (i.e., $\Omega(\boldsymbol{\theta}) = \Omega(\boldsymbol{w})$), where $\boldsymbol{w}$ indicates all the weights
  - Regularizing biases doesn't give much generalization benefit and can lead to significant underfitting
- Sometimes, each layer has a specific coefficient $\lambda^{(i)}$; this increases the number of hyperparameters though

Parameter Norm Penalties (2)

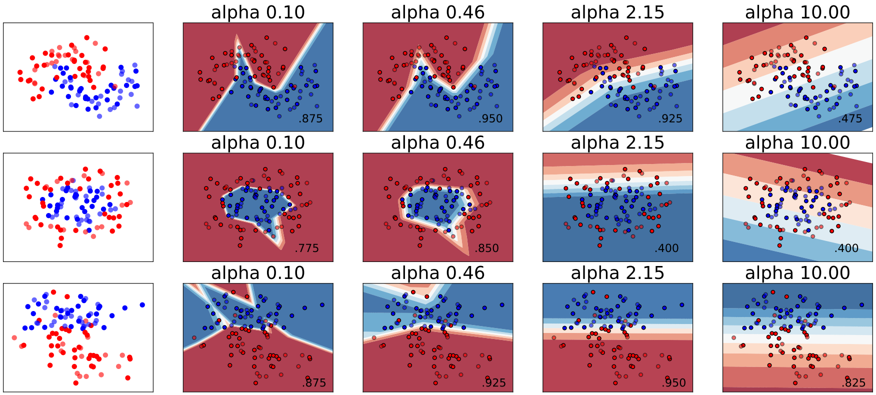
- The most popular choice for the norm penalty is the L^2 norm

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2} \| \boldsymbol{w} \|_2^2$$

- An alternative choice is the L^1 norm

$$\Omega(\boldsymbol{\theta}) = \| \boldsymbol{w} \|_1$$

Example



https://scikit-learn.org/stable/auto_examples/neural_networks/plot_mlp_alpha.html#sphx-glr-auto-examples-neural-networks-plot-mlp-alpha-py

L1/L2 Regularizers in TF

- Regularization terms can be specified per layer
- `kernel_regularizer` affects weights
- `bias_regularizer` affects bias terms

```
from keras import regularizers

layer = layers.Dense(5,
    kernel_regularizer=regularizers.L1(0.01),
    bias_regularizer=regularizers.L2(0.01))
```

Dataset Augmentation

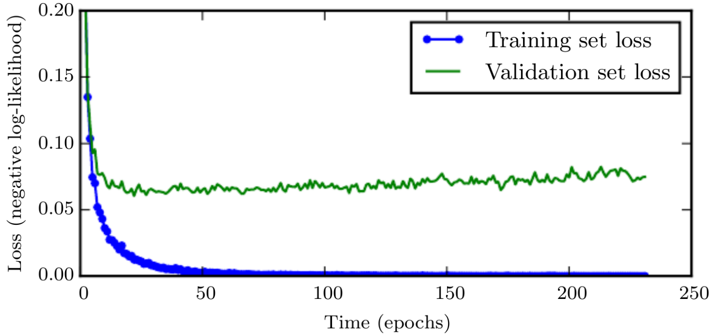
- The best way to make a model generalize better is to train it on more data. Of course, in practice, the amount of data we have is limited...
- Sometimes we are able to create fake data and add it to the training set
- Whether it is possible/easy depends on the task
- Example: in object recognition, we may generate new input images by rotating/translating the existing ones

Noise Injection

- To better generalize, we would like to have NNs that are robust with respect to noise in the input
- As a form of regularization, it can be useful to artificially inject noise when training the NN
  - To the inputs (can be seen as a form of dataset augmentation!)
  - To the weights (e.g., `keras.layers.NoisyDense`)
  - To the hidden units (e.g., `keras.layers.GaussianNoise`)

Early Stopping

- When training large NNs, the model has usually sufficient capacity to overfit the task
- Consider what can happen during training:



Idea: pick the parameters with lowest validation error

Early Stopping meta-algorithm

```
Data: $n$: steps between evaluations
Data: $P$: times validation error worsens before giving up
Data: $\theta_0$: initial parameters
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}_0, \boldsymbol{\theta}^* \leftarrow \boldsymbol{\theta}$
$i, i^*, j \leftarrow 0, v \leftarrow \infty$
while $j < P$ do
    Update $\boldsymbol{\theta}$ running the training alg. for $n$ steps
    $i \leftarrow i + n, j \leftarrow j + 1$
    $v' \leftarrow \text{ValidationError}(\boldsymbol{\theta})$
    if $v' < v$ then
        $j \leftarrow 0$
        $\boldsymbol{\theta}^* \leftarrow \boldsymbol{\theta}$
        $i^* \leftarrow i$
        $v \leftarrow v'$
    end
end
```

Early Stopping (3)

- Likely the most popular form of regularization in DL
  - It can also be used in conjunction with other techniques
- You can view the "training time" as a hyperparameter, which is automatically tuned through early stopping
- In principle, you also enjoy a computational benefit, as the training procedure is shortened
- However, there is the extra cost of repeatedly evaluating the validation error
  - Could be done in parallel with training on a different processor, machine, ...
- Memory overhead due to storage of multiple parameters

Early Stopping (4)

- Early stopping requires the creation of a validation set, which reduces the amount of data available for training
- To exploit the extra data, one may want to perform extra training *after* initial training with early stopping
- Common approach: re-train from scratch with whole dataset, for the number of steps determined by early stopping
- Alternative (more challenging): keep the best parameters and continue training for some (how many?!) steps with all the data

Early Stopping in TensorFlow

- Built-in callback for early stopping
  - monitor: metrics to monitor (e.g., 'loss', 'val_loss')
  - min_delta: minimum change to qualify as an improvement
  - patience: allowed epochs with no improvement

```
callback = keras.callbacks.EarlyStopping(\
        monitor='val_loss', patience=3)
# ...
history = model.fit(..., epochs=10,
              batch_size=16,
              callbacks=[callback])
```

Bagging

- Bagging reduces generalization error combining several models
- The techniques you studied in the first part of the course can be applied to NNs as well
- NNs reach a wide enough variety of solution points that you can often train several models on the same data with minimal changes (e.g., initial weights, minibatch selection, ...)

Dropout

- Dropout is a computationally inexpensive yet powerful method to regularize a broad family of models
  - *Srivastava, Hinton, et al., "Dropout: a simple way to prevent neural networks from overfitting", 2014*
- Can be regarded as an efficient approximation of bagging with exponentially many NNs
- Key idea: dropping out some of the units in the NN randomly
- A different sampled NN is used for every training step

Dropout (2)

- Let $p^{(\ell)} \in (0,1)$ the dropout probability for layer ℓ
  - usually 0.8 for input layer, and 0.5 for hidden units
- Let $\boldsymbol{h}^{(\ell)}$ the output of the ℓ-th layer (where $\boldsymbol{h}^{(0)} = \boldsymbol{x}$)
- For the i-th unit in layers 0, 1, …, $(\ell - 1)$, at every training step we have:

$$\tilde{h}_i^{(\ell)} = \begin{cases} h_i^{(\ell)} & \text{with probability } p \\ 0 & \text{with probability } (1-p) \end{cases}$$

- It's like using a different NN (with shared parameters) for every example in the training set
- After training, we can use the NN *without* dropout, scaling the weights: $\boldsymbol{W}_{test}^{(\ell)} = p^{(\ell)} \boldsymbol{W}^{(\ell)}$

Dropout in TensorFlow

- Dropout available as a layer in Keras
- The Dropout layer randomly sets its **input** units to 0 with a frequency of `rate` at each step **during training** (
- Inputs not set to 0 are scaled up by `1/(1 - rate)` such that the sum over all inputs is unchanged
  - Keras performs input scaling during training as well
  - Slightly different than scaling weights only after training (as described before), but equivalent in practice

```
layer = tf.keras.layers.Dropout(0.5,
                    input_shape=(2,))
```

Optimization Algorithms for NNs

Training

- ML largely relies on mathematical optimization and, especially, gradient-based optimization
- Training large NNs is a challenging task, which can take days or months using 100+ machines
- It is not surprising that specialized optimization techniques have been studied for this problem
- We will briefly review some of these techniques
  - note that an exhaustive and rigorous discussion of the optimization issues in ML is out of the scope of the lectures

Learning vs. Pure Optimization

- Important differences between ML and pure optimization
- The main one: ML acts indirectly
- In pure optimization, given an objective J, you try to minimize J and evaluate a solution based on the value of J
- In ML, you care about a performance measure P defined w.r.t. the test set and possibly intractable
- Therefore, you optimize a different cost function J w.r.t. the training set, hoping that doing so will improve P
- Furthermore, ML training does not stop at (local) minima, but usually when a convergence criterion is met (e.g., early stopping)

Challenges in NN Optimization

- Optimization is difficult; many ML models have been carefully designed to deal with convex optimization problems (which can be still challenging!)
  - Finding a local minimum is enough (it will be a global minimum)
- When training NNs, we must confront the general nonconvex case

Local Minima and Saddle Points

- Deep models guaranteed to have an extremely large number of local minima
- Problematic if they have cost higher than global minimum
- So, are local minima a major problem in NN training?
  - Still an open research question (difficult to establish in high-dimensional spaces)
  - Today, we suspect that, for large NNs, most local minima have a low cost function value

Local Minima and Saddle Points

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  - Still an open research question (difficult to establish in high-dimensional spaces)
  - Today, we suspect that, for large NNs, most local minima have a low cost function value
- For high-dimensional nonconvex functions, more saddle points than local minima
  - Local minimum *and* maximum along different cross-sections
  - Zero gradient, and very small around the point
  - SGD seems quite good at escaping

Vanishing and Exploding Gradients

- Suppose that a computational graph contains a path where a matrix $\boldsymbol{W}$ is repeatedly multiplied
- After t steps, it is equivalent to $\boldsymbol{W}^t$ and for eigendecomposition:

$$\boldsymbol{W}^t = \boldsymbol{V}\text{diag}(\boldsymbol{\lambda})^t\boldsymbol{V}^{-1}$$

- Any eigenvalue λ_i with $|\lambda_i|$ not close to 1 will either vanish or explode, and so the gradients along this graph

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- Mostly regards recurrent NNs, which repeatedly apply the same operation
- Feedforward DNNs use different weights at each layer and can largely avoid the issue

Algorithms

We will see a few algorithms commonly used to train NNs.
We will start from the one you already know, i.e., SGD.

Stochastic Gradient Descent

Stochastic Gradient Descent (SGD) at epoch *k*

```
1 while stopping criterion not met do
2     Sample minibatch $\mathcal{B}$ randomly from the training set
3     $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
4     $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha_k \boldsymbol{g}$
5 end
```

- The learning rate is a crucial paramter for SGD
- So far, we always considered a constant learning rate α
- Let α_k the learning rate at epoch k

SGD: Learning rate

- It is necessary to gradually decrease α_k over time
  - The random selection of samples in SGD introduces noise in gradient estimation, even when we arrive at minimum
- Sufficient conditions for convergence (both must hold):

$$\sum_{k=1}^{\infty} \alpha_k = \infty \qquad \sum_{k=1}^{\infty} \alpha_k^2 < \infty$$

- Common approach: linearly decaying learning rate

$$\alpha_k = \begin{cases} \alpha_0 - \frac{k}{\tau}(\alpha_0 - \alpha_\tau) & k \leq \tau \\ \alpha_\tau & k > \tau \end{cases}$$

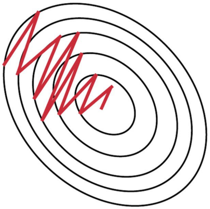
- How to set α_0, α_τ, τ? More of an art than a science…
  - Usually $\alpha_\tau \approx 0.01\alpha_0$
  - Best to look at learning curves

Example: Learning Rate Schedule

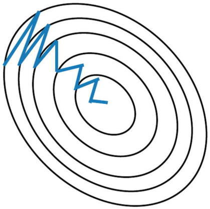
```
s = keras.optimizers\
      .schedules.ExponentialDecay(
    initial_learning_rate=1e-2,
    decay_steps=10000,
    decay_rate=0.9)
opt = keras.optimizers.SGD(learning_rate=s)
```

Momentum

- SGD is a popular choice, but it can be very slow to converge
- The method of momentum aims to accelerate learning
- Idea: accumulate an exponentially decaying moving average of past gradients and continue to move in that direction



Stochastic Gradient
Descent **withhout**
Momentum



Stochastic Gradient
Descent **with**
Momentum

Momentum (2)

- Momentum comes from a physics analogy, in which the negative gradient is a force moving a particle through parameter space
- A variable $\boldsymbol{v}$ plays the role of velocity
    - Actually, in physics, momentum is mass times velocity (with unit mass, $\boldsymbol{v}$ represents momentum)
- A hyperparameter $\beta \in [0, 1)$ determines how fast past contributions decay

Momentum (3)

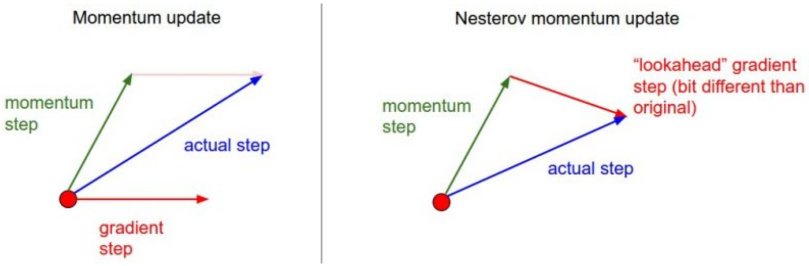
Stochastic Gradient Descent (SGD) with momentum

```
1 while stopping criterion not met do
2     Sample minibatch $\mathcal{B}$ randomly from the training set
3     $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|}\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
4     Update velocity: $\boldsymbol{v} \leftarrow \beta \boldsymbol{v} - \alpha_k \boldsymbol{g}$
5     $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
6 end
```

- SGD step size depends on length and “alignment” of gradient sequence
- Common values for β: 0.5, 0.9, 0.99
- Keras: `SGD(momentum=beta,...)`:

Nesterov Momentum

- Variant of the momentum algorithm
- Adds a correction by evaluating gradient *after* applying the current velocity



Nesterov Momentum (2)

Stochastic Gradient Descent (SGD) with Nesterov momentum

```
1 while stopping criterion not met do
2     Sample minibatch $\mathcal{B}$ randomly from the training set
3     Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \beta \boldsymbol{v}$
4     $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|} \nabla_{\boldsymbol{\theta}} J(\tilde{\boldsymbol{\theta}})$
5     Update velocity: $\boldsymbol{v} \leftarrow \beta \boldsymbol{v} - \alpha_k \boldsymbol{g}$
6     $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
7 end
```

- Keras: `SGD(momentum=beta, nesterov=True, ...)`[1]

[1]The actual implementation is an approximation of Nesterov Momentum, see: `https://stackoverflow.com/a/50778921`

More Algorithms...

- Learning rate is one of the most difficult to set hyperparameters
- Momentum can mitigate some issues, but introduces another hyperparameter
- Idea: using a separate learning rate for each parameter and automatically adapt them

AdaGrad

- Adapt individual learning rate of all model params
- Scaling inversely proportional to square root of the sum of all the historical squared values of the gradient
- "Larger derivatives lead to more rapid decrease"
- AdaGrad has good theoretical properties for convex settings
- Difficult to use in practice due to gradient storage requirement
  - Still worth presenting because of its extensions!

AdaGrad: Algorithm

AdaGrad

```
r ← 0                                  /* Gradient accumulation */
while stopping criterion not met do
    Sample minibatch $\mathcal{B}$ randomly from the training set
    $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|}\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
    $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + -\frac{\alpha}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$
end
```

Notes:

- $\odot$ denotes element-wise operations
- δ is a small positive constant (usually 10^{-7})

RMSProp

- Proposed by Hinton in 2012, RMSProp (Root Mean Squared Propagation) modifies AdaGrad
- One of the most used optimization algorithms for DNNs
- Gradient accumulation becomes an exponentially moving average
  - Nonconvex problems better handled
  - No need to store all the gradients
- New hyperparameter ρ: length scale of the moving average

RMSProp: Algorithm

RMSProp

```
1 $\boldsymbol{r} \leftarrow 0$                              /* Gradient accumulation */
2 while stopping criterion not met do
3     Sample minibatch $\mathcal{B}$ randomly from the training set
4     $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|}\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
5     $\boldsymbol{r} \leftarrow \rho\boldsymbol{r} + (1-\rho)\boldsymbol{g} \odot \boldsymbol{g}$
6     $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + -\frac{\alpha}{\delta+\sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$
7 end
```

Notes:

- $\odot$ denotes element-wise operations
- δ is a small positive constant (usually 10^{-6})

RMSProp: Algorithm (2)

RMSProp with Nesterov momentum

```
1 $\boldsymbol{r} \leftarrow 0$                    /* Gradient accumulation */
2 **while** *stopping criterion not met* **do**
3     Sample minibatch $\mathcal{B}$ randomly from the training set
4     Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \beta \boldsymbol{v}$
5     $\boldsymbol{g} \leftarrow \frac{1}{|\mathcal{B}|} \nabla_{\boldsymbol{\theta}} J(\tilde{\boldsymbol{\theta}})$
6     $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho) \boldsymbol{g} \odot \boldsymbol{g}$
7     $\boldsymbol{v} \leftarrow \beta \boldsymbol{v} - \frac{\alpha}{\sqrt{r}} \odot \boldsymbol{g}$
8     $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
9 **end**
```

Adam

- Proposed in 2014, Adam ("adaptive moments") can be seen as a variant of RMSProp with momentum
- Adam computes individual adaptive learning rates for different parameters from estimates of first and second moments of the gradients
- Important differences w.r.t. RMSProp:
    - Momentum directly incorporated as an estimate of the first-order moment of the gradient (while in RMSProp is applied to rescaled gradient, without theoretical justification)
    - Estimates of the first- and second-order moments are corrected to avoid initialization bias (moving averages are initialized as 0)

Choosing the Algorithm

- How to choose the algorithm to use?
- No single answer!

- The algorithms we have discussed are popular choices
- User's familiarity with the algorithm is an important factor in the choice
  - If you are not familiar, difficult to tune hyperparameters

Parameter Initialization

- How parameters are initialized determines the initial point (in the parameter space) where the optimization starts
- The initial point can determine whether the algorithm converges at all!
  - some initial points are so unstable that the algorithm encounters numerical difficulties
- When learning does converge, the initial point can determine converge speed and whether a point with high or low cost is reached
- Various heuristics proposed, usually random-based

Parameter Initialization (2)

- Random Normal/Uniform: sample weights randomly from a given distribution
- Xavier[2] method: now almost a standard practice
  - weights randomly sampled from a Gaussian distribution
  - $\mu = 0$
  - $\sigma^2 = \frac{2}{n_{IN}+n_{OUT}}$, where n_{IN} and n_{OUT} denote the number of inputs and outputs in the layer

```
init = keras.initializers.GlorotNormal()
layer = keras.layers.Dense(3,
                    kernel_initializer=init)
```

[2]Named after Xavier Glorot, who proposed the method with Bengio

Batch Normalization

- Batch normalization (BN) is a popular and effective technique to accelerate the convergence of deep NNs
  - Not an optimization algorithm, but a tool to improve convergence
  - Regularization effect as a secondary benefit
  - Proposed in 2015
- BN is applied to individual layers (or, possibly, to all of them)
- Input re-scaling and standardization benefits optimizers, since it puts the parameters on a similar scale
- It is natural to ask whether a similar normalization step inside a NN might be beneficial

Batch Normalization (2)

- Consider a minibatch $\mathcal{B}$ and an input $\boldsymbol{x} \in \mathcal{B}$

$$BN(\boldsymbol{x}) = \frac{\boldsymbol{x} - \hat{\boldsymbol{\mu}}_{\mathcal{B}}}{\hat{\boldsymbol{\sigma}}_{\mathcal{B}}}$$

  where $\hat{\boldsymbol{\mu}}_{\mathcal{B}}$ and $\hat{\boldsymbol{\sigma}}_{\mathcal{B}}$ denote the mean and std. deviation of the minibatch. (Note: they are vectors with the same shape of $\boldsymbol{x}$)
- The resulting minibatch has zero mean and unit variance

Batch Normalization (3)

- In practice, BN is applied to hidden layers

$\boldsymbol{h} = \phi(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$ becomes $\boldsymbol{h} = \phi(BN(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}))$

- The expression above follows the original paper presenting BN; actually, implementations often apply BN *after* the activation function

$$\boldsymbol{h} = BN(\phi(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}))$$

Batch Normalization (4)

- Layer activations seem to be limited in their expressive power (e.g., they are forced to have unit variance)
- A more general BN formulation:

$$BN(\boldsymbol{x}) = \gamma \frac{\boldsymbol{x} - \hat{\boldsymbol{\mu}}_{\mathcal{B}}}{\hat{\boldsymbol{\sigma}}_{\mathcal{B}}} + \boldsymbol{\beta}$$

  where the *vectors* γ and $\boldsymbol{\beta}$ are parameters to learn as part of training

Batch Normalization (4)

- Layer activations seem to be limited in their expressive power (e.g., they are forced to have unit variance)
- A more general BN formulation:

$$BN(\boldsymbol{x}) = \gamma \frac{\boldsymbol{x} - \hat{\mu}_{\mathcal{B}}}{\hat{\sigma}_{\mathcal{B}}} + \boldsymbol{\beta}$$

  where the *vectors* γ and $\boldsymbol{\beta}$ are parameters to learn as part of training
- Question: why did we force the mean to be zero and now introduce a parameter to allow for any mean??
  - We can represent the same family of functions as before, but now we have different (and easier!) learning dynamics
  - Mean and variance solely depend on γ and $\boldsymbol{\beta}$, whilst without BN they depend on the complicated interaction of the parameters in all the previous layers!

Batch Normalization (5)

- The formulas presented so far describe how BN works during training
- The behavior is slightly different at inference time, because it must be able to work without minibatches (e.g., prediction against a single input value)
  - Question: what happens if you apply BN as described so far to a minibatch of size 1?
- At inference time, normalization uses a moving average of the mean and standard deviation of the minibatches seen during training

Batch Normalization in Keras

- It is extremely easy to integrate BN in Keras
- It is offered as specific type of layer, to be used *after* the hidden layer where it must be applied:

```
model = keras.Sequential()
model.add(layers.Dense(16))
model.add(layers.BatchNormalization())
```