

Batch Normalization

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Feature Scaling for Linear Models

Why Feature Scaling?

People's feature vectors: $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^2$.

- The 1st dimension is one person's income (**in dollars**).
 - Assume it is randomly from the Gaussian distribution $N(3000, 400^2)$.
- The 2nd dimension is one person's height (**in inch**).
 - Assume it is randomly from the Gaussian distribution $N(69, 3^2)$.

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 - Assume it is randomly from the Gaussian distribution $N(69, 3^2)$.

- Hessian matrix of least squares regression model:

$$\mathbf{H} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T = \begin{bmatrix} 9137.3 & 206.6 \\ 206.6 & 4.8 \end{bmatrix} \times 10^3.$$

- Condition number: $\frac{\lambda_{\max}(\mathbf{H})}{\lambda_{\min}(\mathbf{H})} = 9.2 \times 10^4$.

Bad condition number means slow convergence of gradient descent!

Why Feature Scaling?

People's feature vectors: $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^2$.

- The 1st dimension is one person's income (**in thousand dollars**).
 - Assume it is randomly from the Gaussian distribution $N(3, 0.4^2)$.
- The 2nd dimension is one person's height (**in foot**).
 - Assume it is randomly from the Gaussian distribution $N(5.75, 0.25^2)$.

- **Change metric.**

- Hessian matrix of linear regression:

$$\mathbf{H} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T = \begin{bmatrix} 9.1 & 17.2 \\ 17.2 & 33.1 \end{bmatrix}.$$

- Condition number: $\frac{\lambda_{\max}(\mathbf{H})}{\lambda_{\min}(\mathbf{H})} = 281.7$. (As opposed to 92K.)

Feature Scaling for **1D** Data

Assume the samples x_1, \dots, x_n are **one-dimensional**.

- **Min-max normalization:** $x'_i = \frac{x_i - \min(x_i)}{\max(x_i) - \min(x_i)}$.
- After the scaling, the samples x'_1, \dots, x'_n are in $[0, 1]$.

Feature Scaling for **1D** Data

Assume the samples x_1, \dots, x_n are **one-dimensional**.

- **Standardization:** $x'_i = \frac{x_i - \hat{\mu}}{\hat{\sigma}}$.
 - $\hat{\mu} = \frac{1}{n} \sum_{i=1}^n x_i$ is the sample mean.
 - $\hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \hat{\mu})^2$ is the sample variance.
 - After the scaling, the samples x'_1, \dots, x'_n have zero mean and unit variance.

Feature Scaling for **High-Dim** Data

- Independently perform feature scaling for every feature.
 - E.g., when scaling the “height” feature, ignore the “income” feature.

```
# Min-Max Normalization
```

```
import numpy
```

```
d = x.shape[1]
```

```
xmin = numpy.min(x, axis=0).reshape(1, d)
```

```
xmax = numpy.max(x, axis=0).reshape(1, d)
```

```
xnew = (x - xmin) / (xmax - xmin)
```


Feature Scaling for **High-Dim** Data

- Independently perform feature scaling for every feature.
 - E.g., when scaling the “height” feature, ignore the “income” feature.

```
# Standardization
```

```
import numpy
```

```
d = x.shape[1]
```

```
mu = numpy.mean(x, axis=0).reshape(1, d)
```

```
sig = numpy.std(x, axis=0).reshape(1, d)
```

```
xnew = (x - mu) / sig
```

Batch Normalization

Batch Normalization: Standardization of Hidden Layers

- Let $\mathbf{x}^{(k)} \in \mathbb{R}^d$ be the output of the k -th hidden layer.
- $\hat{\boldsymbol{\mu}} \in \mathbb{R}^d$: sample mean of $\mathbf{x}^{(k)}$ evaluated on a batch of samples.
- $\hat{\boldsymbol{\sigma}} \in \mathbb{R}^d$: sample std of $\mathbf{x}^{(k)}$ evaluated on a batch of samples.

- Standardization: $z_j^{(k)} = \frac{x_j^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.

Batch Normalization: Standardization of Hidden Layers

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- $\hat{\boldsymbol{\mu}} \in \mathbb{R}^d$: sample mean of $\mathbf{x}^{(k)}$ evaluated on a batch of samples.
- $\hat{\boldsymbol{\sigma}} \in \mathbb{R}^d$: sample std of $\mathbf{x}^{(k)}$ evaluated on a batch of samples.
- $\boldsymbol{\gamma} \in \mathbb{R}^d$: scaling parameter (trainable).
- $\boldsymbol{\beta} \in \mathbb{R}^d$: shifting parameter (trainable).
- Standardization: $z_j^{(k)} = \frac{x_j^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.
- Scale and shift: $x_j^{(k+1)} = z_j^{(k)} \circ \gamma_j + \beta_j$, for $j = 1, \dots, d$.

Batch Normalization: Standardization of Hidden Layers

- Let $\mathbf{x}^{(k)} \in \mathbb{R}^d$ be the output of the k -th hidden layer.
- $\hat{\boldsymbol{\mu}} \in \mathbb{R}^d$: **Non-trainable**. Just record them in the forward pass;
- $\hat{\boldsymbol{\sigma}} \in \mathbb{R}^d$: use them in the backpropagation.
- $\boldsymbol{\gamma} \in \mathbb{R}^d$: scaling parameter (**trainable**).
- $\boldsymbol{\beta} \in \mathbb{R}^d$: shifting parameter (**trainable**).
- Standardization: $z_j^{(k)} = \frac{x_j^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.
- Scale and shift: $x_j^{(k+1)} = z_j^{(k)} \circ \gamma_j + \beta_j$, for $j = 1, \dots, d$.

Backpropagation for Batch Normalization Layer

- Standardization: $z^{(k)} = \frac{x^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.
- Scale and shift: $x^{(k+1)} = z^{(k)} \circ \gamma_j + \beta_j$, for $j = 1, \dots, d$.

We know $\frac{\partial L}{\partial x^{(k+1)}}$ from the backpropagation (from the top to $x^{(k+1)}$.)

- Use $\frac{\partial L}{\partial \gamma_j} = \frac{\partial L}{\partial x^{(k+1)}} \frac{\partial x^{(k+1)}}{\partial \gamma_j} = \frac{\partial L}{\partial x^{(k+1)}} z^{(k)}$ to update γ_j ;
- Use $\frac{\partial L}{\partial \beta_j} = \frac{\partial L}{\partial x^{(k+1)}} \frac{\partial x^{(k+1)}}{\partial \beta_j} = \frac{\partial L}{\partial x^{(k+1)}}$ to update β_j .

Backpropagation for Batch Normalization Layer

- Standardization: $z^{(k)} = \frac{x^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.
- Scale and shift: $x^{(k+1)} = z^{(k)} \circ \gamma_j + \beta_j$, for $j = 1, \dots, d$.

We know $\frac{\partial L}{\partial x^{(k+1)}}$ from the backpropagation (from the top to $x^{(k+1)}$.)

Compute $\frac{\partial L}{\partial z^{(k)}} = \frac{\partial L}{\partial x^{(k+1)}} \frac{\partial x^{(k+1)}}{\partial z^{(k)}} = \frac{\partial L}{\partial x^{(k+1)}} \gamma_j$.

Compute $\frac{\partial L}{\partial x^{(k)}} = \frac{\partial L}{\partial z^{(k)}} \frac{\partial z^{(k)}}{\partial x^{(k)}} = \frac{\partial L}{\partial z^{(k)}} \frac{1}{\hat{\sigma}_j + 0.001}$ and pass it to the lower layers.

Batch Normalization Layer in Keras

Batch Normalization Layer

- Let $\mathbf{x}^{(k)} \in \mathbb{R}^d$ be the output of the k -th hidden layer.
- $\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\sigma}} \in \mathbb{R}^d$: **non-trainable** parameters.
- $\boldsymbol{\gamma}, \boldsymbol{\beta} \in \mathbb{R}^d$: **trainable** parameters.
- Standardization: $z_j^{(k)} = \frac{x_j^{(k)} - \hat{\mu}_j}{\hat{\sigma}_j + 0.001}$, for $j = 1, \dots, d$.
- Scale and shift: $x_j^{(k+1)} = z_j^{(k)} \cdot \gamma_j + \beta_j$, for $j = 1, \dots, d$.

Batch Normalization Layer

- Let $\mathbf{x}^{(k)} \in \mathbb{R}^d$ be the output of the k -th hidden layer.
- $\hat{\mu}, \hat{\sigma} \in \mathbb{R}^d$: **non-trainable** parameters.
- $\gamma, \beta \in \mathbb{R}^d$: **trainable** parameters.

Difficulty: There are $4d$ parameters which must be stored in memory.
 d can be very large!

Example:

- The 1st Conv Layer in VGG16 Net outputs a $150 \times 150 \times 64$ tensor.
- The number of parameters in a single Batch Normalization Layer would be $4d = 1.44\text{M}$.

Batch Normalization Layer

Solution:

- Make the 4 parameters $1 \times 1 \times 64$, instead of $150 \times 150 \times 64$.
- How?
- A scalar parameter for a slice (e.g., a 150×150 matrix) of the tensor.
- Of course, you can make the parameters $150 \times 1 \times 1$ or $1 \times 150 \times 1$.

Example:

- The 1st Conv Layer in VGG16 Net outputs a $150 \times 150 \times 64$ tensor.
- The number of parameters in a single Batch Normalization Layer would be $4d = 1.44\text{M}$.

CNN for Digit Recognition

```
from keras import models
from keras import layers

model = models.Sequential()
model.add(layers.Conv2D(10, (5, 5), input_shape=(28, 28, 1)))
model.add(layers.BatchNormalization())
model.add(layers.Activation('relu'))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(20, (5, 5)))
model.add(layers.BatchNormalization())
model.add(layers.Activation('relu'))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Flatten())
model.add(layers.Dense(100))
model.add(layers.BatchNormalization())
model.add(layers.Activation('relu'))
model.add(layers.Dense(10, activation='softmax'))
```

CNN for Digit Recognition

Layer (type)	Output Shape	Param #
conv2d_1 (Conv2D)	(None, 24, 24, 10)	260
batch_normalization_1 (Batch Normalization)	(None, 24, 24, 10)	40
activation_1 (Activation)	(None, 24, 24, 10)	0
max_pooling2d_1 (MaxPooling2D)	(None, 12, 12, 10)	0
conv2d_2 (Conv2D)	(None, 8, 8, 20)	5020
batch_normalization_2 (Batch Normalization)	(None, 8, 8, 20)	80
activation_2 (Activation)	(None, 8, 8, 20)	0
max_pooling2d_2 (MaxPooling2D)	(None, 4, 4, 20)	0
flatten_1 (Flatten)	(None, 320)	0
dense_1 (Dense)	(None, 100)	32100
batch_normalization_3 (Batch Normalization)	(None, 100)	400
activation_3 (Activation)	(None, 100)	0
dense_2 (Dense)	(None, 10)	1010
Total params: 38,910		
Trainable params: 38,650		
Non-trainable params: 260		

CNN for Digit Recognition

Train the model (**with** Batch Normalization) on MNIST ($n = 50,000$).

Train on 50000 samples, validate on 10000 samples

Epoch 1/3

50000/50000 [=====] - 29s 580us/step -
loss: 0.1599 - acc: 0.9595 - val_loss: 0.1165 - val_acc: 0.9644

Epoch 2/3

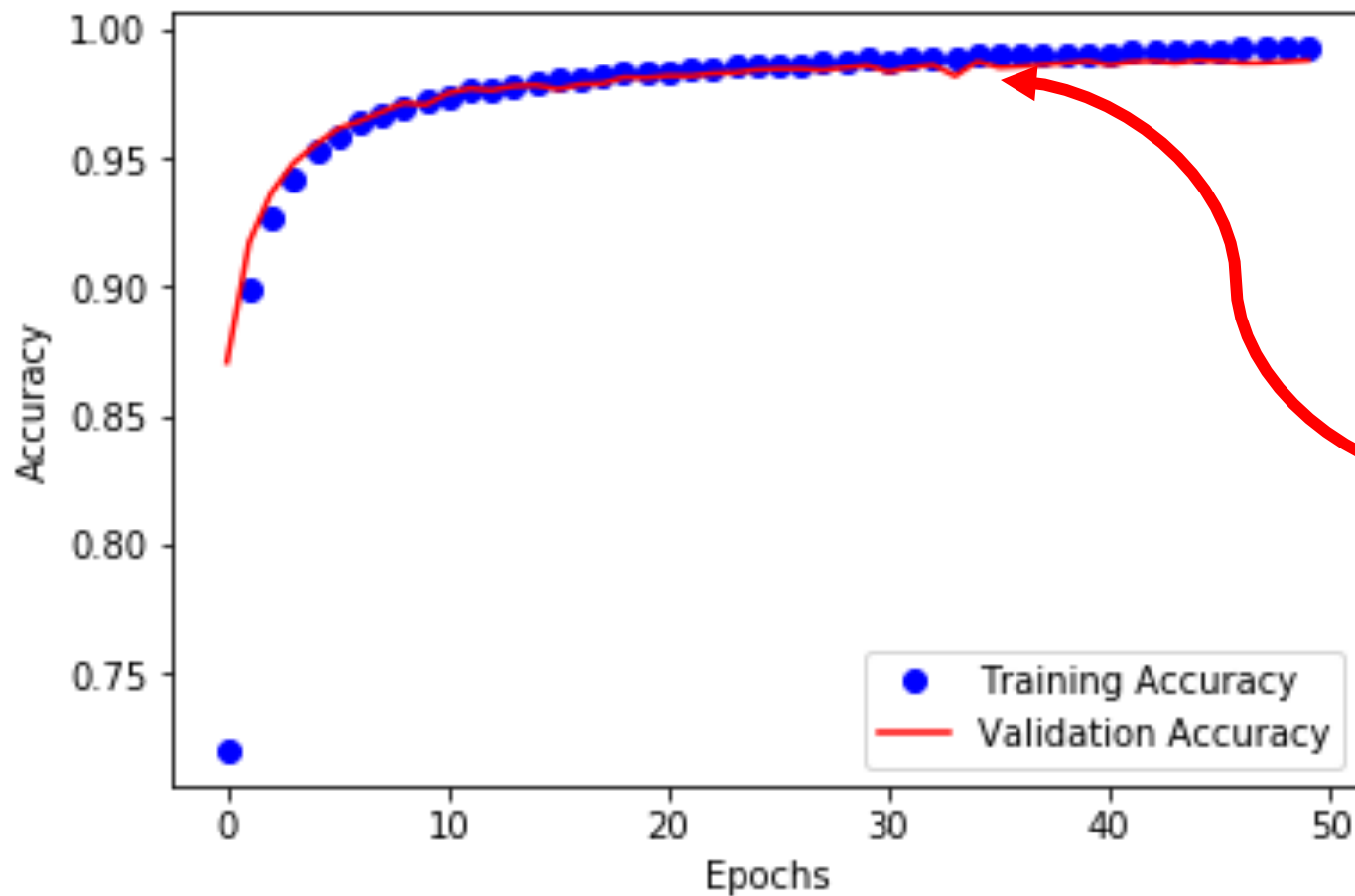
50000/50000 [=====] - 26s 516us/step -
loss: 0.0468 - acc: 0.9858 - val_loss: 0.0562 - val_acc: 0.9822

Epoch 3/3

50000/50000 [=====] - 25s 508us/step -
loss: 0.0325 - acc: 0.9902 - val_loss: 0.0494 - val_acc: 0.9832

CNN for Digit Recognition

Train the model (**without** Batch Normalization) on MNIST ($n = 50,000$).



Without Batch Normalization,
it takes 10x more epochs to
converge.

Summary

Feature Scaling

- Make the scales of all the features comparable.
- Why? Better conditioned Hessian matrix → Faster convergence.

Feature Scaling

- Make the scales of all the features comparable.
- Why? Better conditioned Hessian matrix → Faster convergence.
- Methods:
 - Min-Max Normalization: scale the features to $[0, 1]$.
 - Standardization: every feature has zero mean and unit variance.

Batch Normalization

- Feature standardization for the hidden layers.
- Why? Faster convergence.
- 2 trainable parameters: shifting and scaling.
- 2 non-trainable parameters: mean, variance.

Batch Normalization

- Feature standardization for the hidden layers.
- Why? Faster convergence.
- 2 trainable parameters: `shifting and scaling`.
- 2 non-trainable parameters: `mean, variance`.
- Keras provides `layers.BatchNormalization()`.
- Put the BN layer `after Conv` and `before Activation`.