Regularization

BOSTON UNIVERSITY
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Oct. 10, 2017

Brief Recap: Neural Networks & Gradients

- Neural networks are composition of matrices and non-linear functions
- Train networks on data to approximate functions
- Use gradient descent to search parameter space to minimize cost
- Cost function measures distance between hypothesis and label

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Vectorization in PYTORCH

Create a Random 2x2 Image

```
>> from torch import randn
>> image = randn(2,2)
>> image

 2.3042 -0.3380
-0.2713  0.5415
[torch.FloatTensor of size 2x2]
```

Vectorize Image & Create Class Label

```
>> from torch.autograd import
Variable
>> image = Variable(image.view(1,4))

Variable containing:
 2.3042 -0.3380 -0.2713  0.5415
[torch.FloatTensor of size 1x4]

>> from torch import LongTensor
>> label = Variable(LongTensor([1]))

Variable containing:
 1
[torch.LongTensor of size 1]
```

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MLP in PYTORCH

Define Fully-Connected Network

```
>> import torch.nn as nn
>> net =
nn.Sequential(nn.Linear(4, 2),
nn.Sigmoid(), nn.Linear(2, 2))
>> net
Sequential (
  (0): Linear (4 -> 2)
  (1): Sigmoid ()
  (2): Linear (2 -> 2)
)
```

Feedforward the Feature Vector

```
>> net(image)
Variable containing:
 0.0817  0.3724
[torch.FloatTensor of size 1x2]
```

Define Optimizer

```
>> from torch import optim
>> optimizer =
optim.SGD(net.parameters(), lr=1)
```

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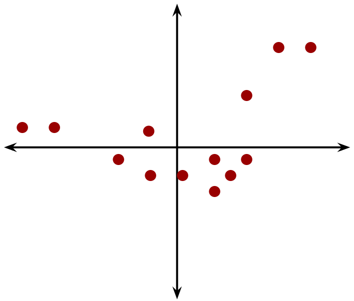
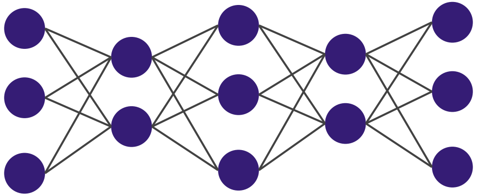
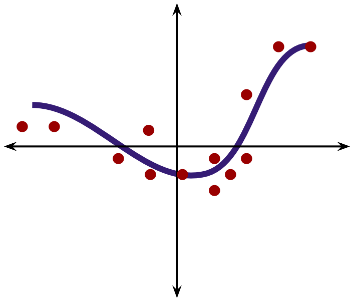
Goal of Learning: Data-Driven Generalization



Dataset



Trained learning algorithm



Approximate function to generalize to new data

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Dataset

Split - percentages depend on available data

Balance - data distributed close to uniformly

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How much data is enough data?

- In practice, the size of real datasets can be on the orders of 10^5, 10^6, 10^7...
- Depends on dimensionality, population, linearity of data

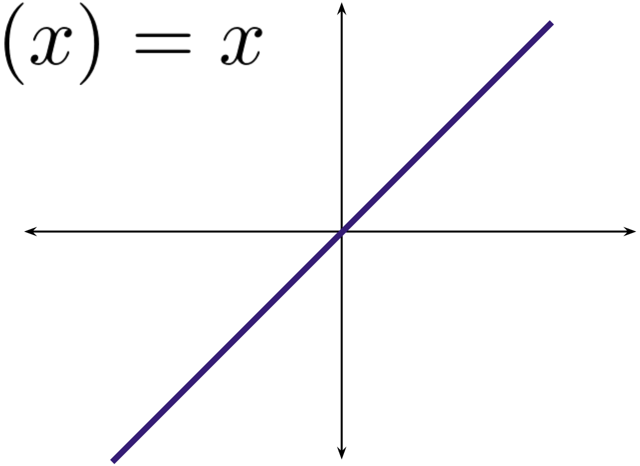
Example:

- Imagine we want to model single pixel images with one color channel
- Each pixel can takes on values in the rangen [0, 255]
- 256 total colors, and in this case 256 total images

How much data is enough data?

- Assume uniform distribution for this example
- Can model with a simple linear classifier over a compact set and only need to collect 256 images to model entire space
- x = 1, f(x) = 1, …

$$f(x) = x$$



$x =$  $f(x) = 254$

$\frac{1}{256}$ $\frac{1}{256}$ $\frac{1}{256}$ $\frac{1}{256}$ … $\frac{1}{256}$ $\frac{1}{256}$ $\frac{1}{256}$

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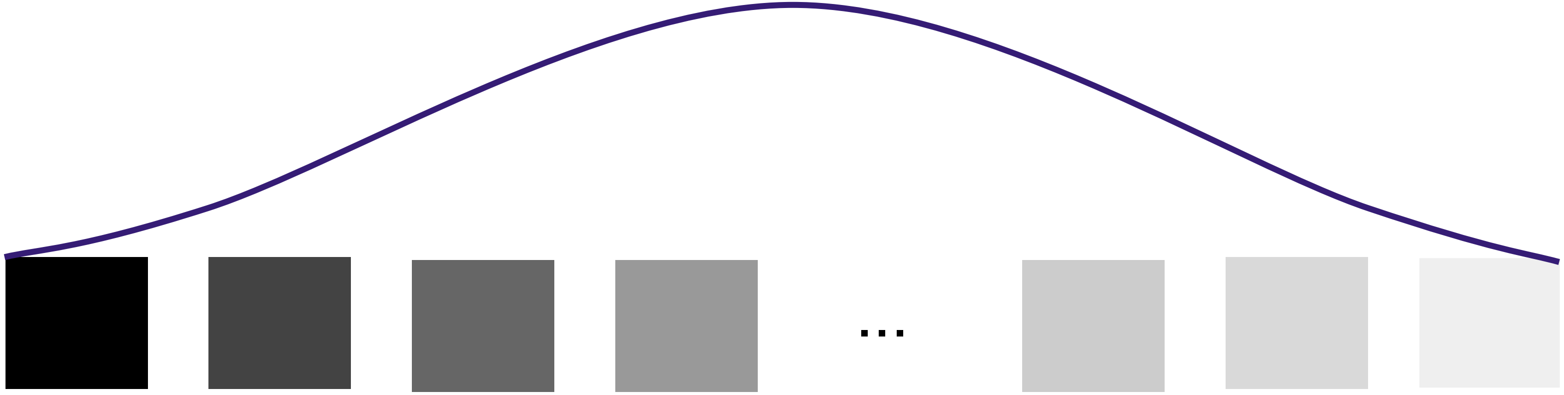
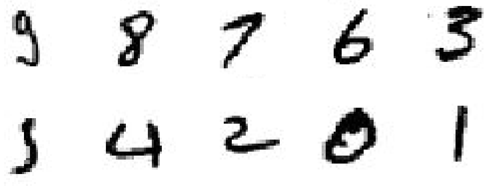
How much data is enough data?

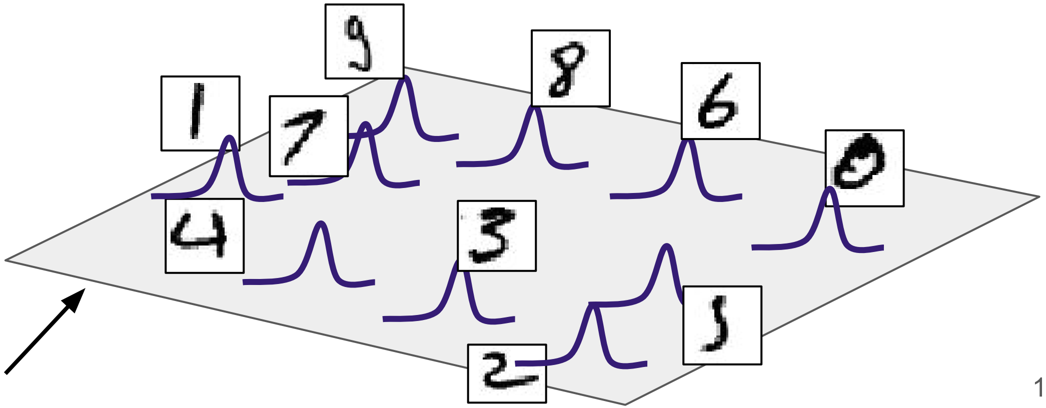
- Now assume Gaussian for this example
- Images towards the center are more likely to occur than those near the tails
- Real images: [117, 137]   21/256 = 8.20% of space
- Random noise: [0, 117) U (137, 255]   235/256 = 91.80% of space



How much data is enough data?

- Now consider 28x28 images with 1 color channel
- 784-dimensional space
- 28 x 28 x 256 x 1 = **200,704 possible images**
- MNIST dataset = 70,000/200,704 = **34.88% of total space**
- **Manifold** = connected regions of space that locally appears Euclidean space





Conceptual illustration of space of possible 28x28x256 images

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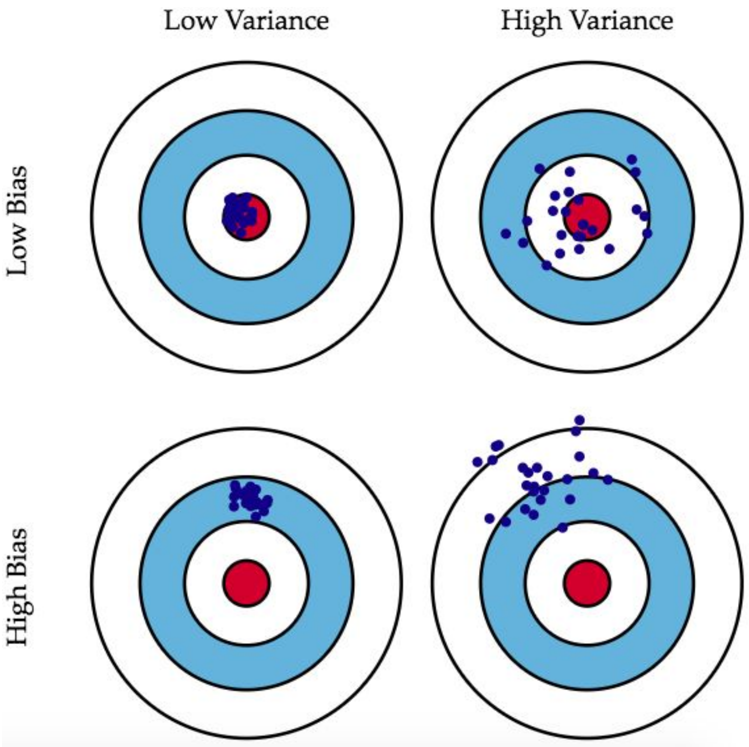
Bias-Variance Tradeoff

- What happens if our dataset is **unbalanced**?
- Learning algorithms are only as good as your data
- **Bias** = concentration around a particular area/ set of points
- **Variance** = spread/distance each point is from each other in an area



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Bias-Variance Tradeoff

Bias **<u>error</u>** says "when you predict things how far are you from the expected **true values**"

$$B = E[f(x;D) - E[y|x]]$$

Variance **<u>error</u>** says "when you predict things how far are you from **other predictions** you've made"

$$V = E[(f(x;D) - E[f(x;D)])^2]$$

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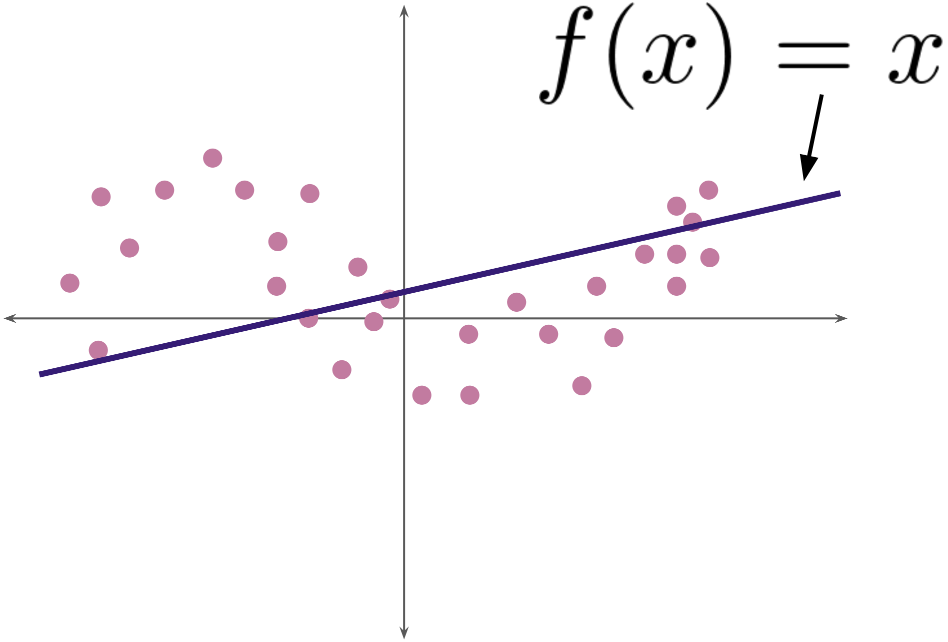
Underfitting

- **High bias error**
- Low **training** <u>**accuracy**</u>
- Low **testing** <u>**accuracy**</u>
- Learning algorithm lacks capacity to model data

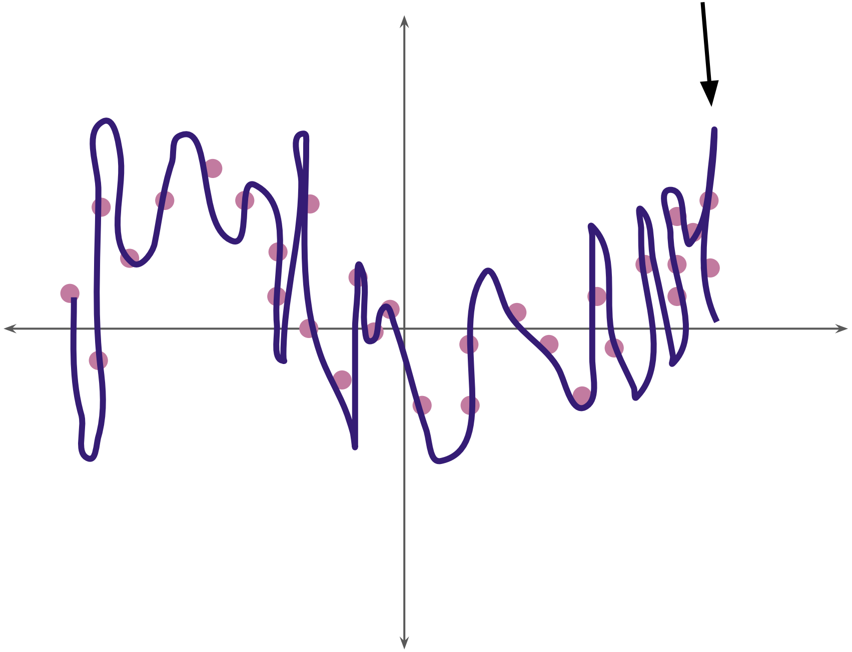


Data from $f(x) = sin(x - \pi)$

Overfitting

$$f(x) = \theta_n x_n^k + \ldots + \theta_0 x_0$$

- **High variance error**
- High **training accuracy**
- Low **testing accuracy**
- Model is **overparameterized**
- Fitting the training set perfectly (**memorization**)



Data from $f(x) = sin(x - \pi)$

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Capacity

- **Representational capacity** - set of hypotheses that can be **expressed** by a trained model's parameters
- **Effective capacity** - set of hypotheses that can be **reached by training** on a particular set of data
- **Model capacity** - number of trainable model parameters

$$\underbrace{EC}_{\text{Effective capacity}}(\underbrace{\mathcal{A}}_{\text{Learning algorithm}}) = \{\underbrace{h}_{\text{Hypothesis}} | \exists \underbrace{\mathcal{D}}_{\text{Dataset}} \ s.t. \ h \in \mathcal{A}(\mathcal{D})\}$$

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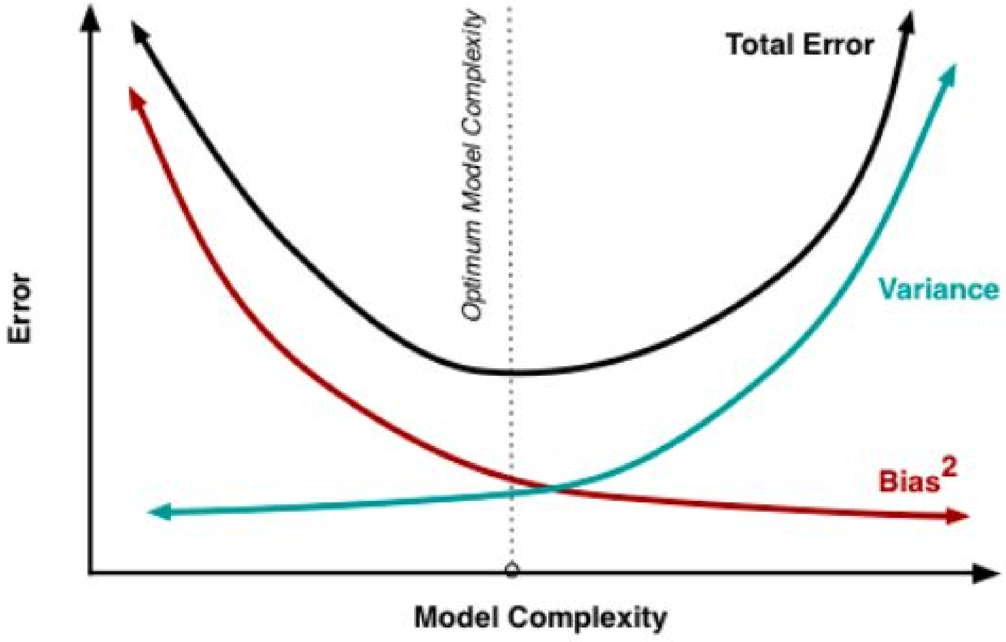
Bias-Variance Tradeoff



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Priors

- A prior knowledge can help generalization
- Independent features
  - Don’t want to over represent features
  - e.g. Modeling house prices
    - Features: length and width of property, and area
- Model selection
  - Selecting an architecture that is better suited for particular data
    - e.g. CNN for compositional data or RNN for sequential data, or logistic classifier for binary classification
- No Free Lunch Theorem
  - There is no single learning algorithm that works best for all problems.

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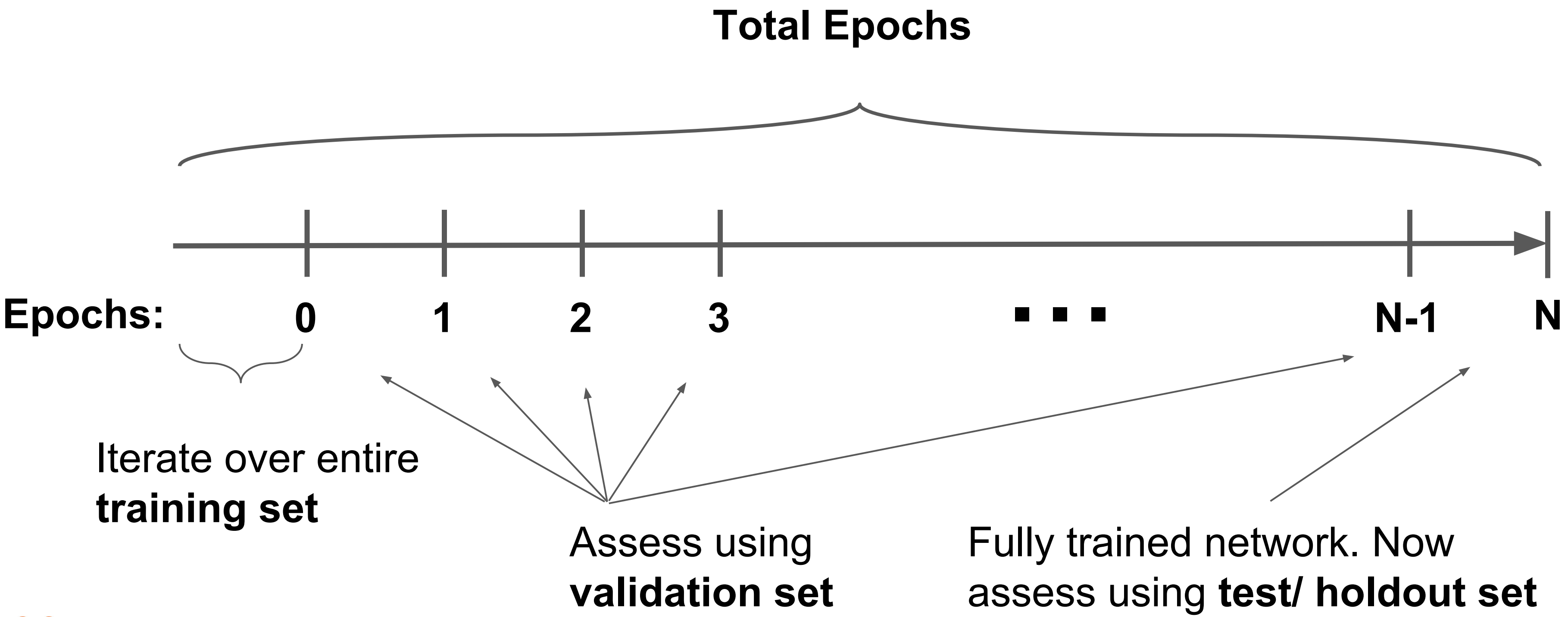
Early Stopping



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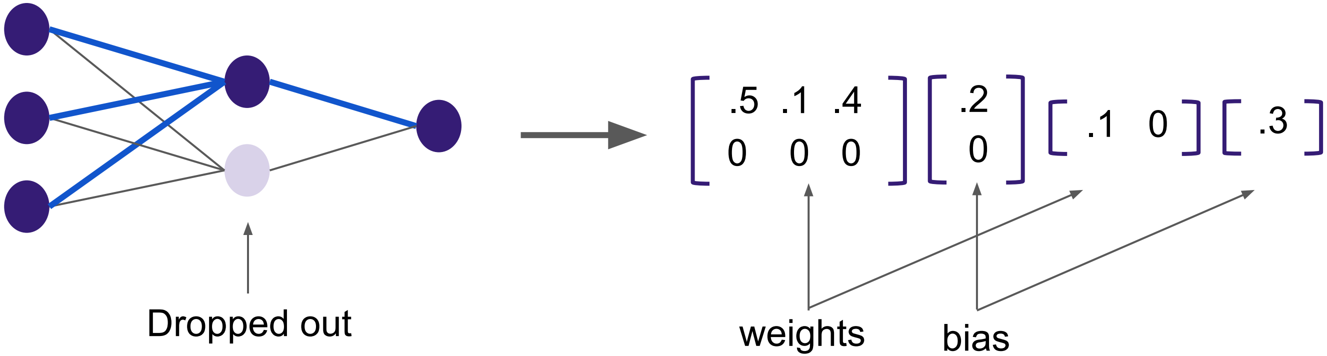
Dropout: A Simple Way to Prevent Neural Networks from Overfitting

- *Srivastava et al*, 2014
- Randomly disable neurons during training with Bernoulli random variable
- Scale output of dropped out of neuron during inference
- Causes networks to become sparse (lots of zeros in matrices)



Co-adaptation

- *Hinton et. al, 2012*
- Co-adaptation - neurons tend to rely on features learned by connected neurons
- To break that adaptation, neurons are dropped during training
- Forces each neuron to try to learn something interesting
- Effectively, learns exponentially many subnetworks that are averaged during inference

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Dropout in PYTORCH

Define Dropout Network

```
>> net = nn.Sequential(nn.Linear(4, 2), nn.Sigmoid(), nn. Dropout(),
nn.Linear(2, 2), nn.Softmax())
>> net
Sequential (
   (0): Linear (4 -> 2)
   (1): Sigmoid ()
   (2): Dropout (p = 0.5)
   (3): Linear (2 -> 2)
   (4): Softmax ()

)
```

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Network Parameter in PYTORCH

```
>> [x for x in net.parameters()]
[Parameter containing:
-0.0046 -0.1379 -0.4034  0.0733
-0.4190  0.1449  0.2962  0.2015
[torch.FloatTensor of size 2x4]
, Parameter containing:
-0.1390
 0.4595
[torch.FloatTensor of size 2]
, Parameter containing:
-0.5009  0.4981
-0.4290  0.6568
[torch.FloatTensor of size 2x2]
, Parameter containing:
-0.4264
-0.3450
[torch.FloatTensor of size 2]
]
```

Layer 1 Weights

Layer 1 Biases

Layer 2 Weights

Layer 2 Biases

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Update Parameters in PYTORCH

Local Gradients

```
>> [x.grad for x in
net.parameters()]
[None, None, None, None]
```

Feedforward

```
>> optimizer.zero_grad()
>> hypo = net(image)
Variable containing:
 0.4322  0.5678
[torch.FloatTensor of size 1x2]
```

Backpropagation

```
>> import torch.nn.functional as F
>> loss = F.nll_loss(hypo, label)
>> loss
Variable containing:
-0.5497
[torch.FloatTensor of size 1]

>> loss.backward()
```

Gradient Descent

```
>> optimizer.step()
```

zero_grad()	Clears the gradients of all optimized variables.
nll_loss()	The negative log likelihood loss
step()	Updates the parameters

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L1 Weight Decay

- Sum the distances between each parameter and the origin
- Sparsifies weight matrices - some weights become zero
- Each of theta is a weight vector - a row in a weight matrix (**neuron**)
- L2 tends to work better in practice

$$L1_{Norm} = \|\theta\|_1 = \sum_i |\theta_i|$$

$$\theta := \theta - \frac{\partial}{\partial \theta}(J(x, y; \theta) + \|\theta\|_1)$$

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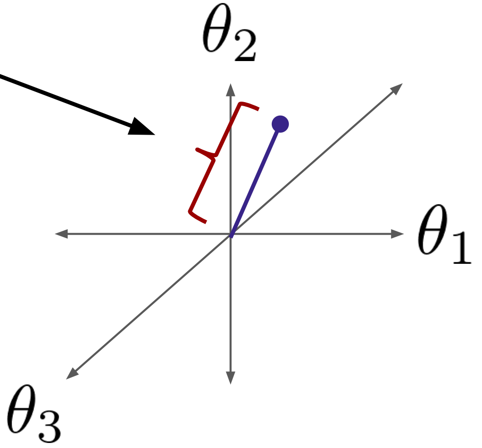
L2 Regularization

- L2-norm a.k.a. Euclidean norm

$$L2_{Norm} = \|\theta\|_2 = \sqrt{\sum_i \theta_i^2}$$

$$\bar{\theta}^\top = [\theta_1 \ \theta_2 \ \theta_3]$$



- L2 regularization a.k.a. weight decay
- Weight decay is L2-norm squared

$$L2_{Reg} = \|\theta\|_2^2 = \sum_i \theta_i^2$$

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L2 Weight Decay

- Add regularization term to cost function
- λ controls how much weights should be decayed
- ½ and square for mathematical convenience
- Pulls all weights towards origin/ zero
- Forces each dimension to contribute

$$\theta := \theta - \frac{\partial}{\partial \theta}\left(J(x, y; \theta) + \frac{\lambda}{2}\|\theta\|_2^2\right)$$

$$\theta := \theta - \frac{\partial}{\partial \theta} J(x, y; \theta) - \lambda\theta$$

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Data Augmentation

- Apply some natural domain-dependent transformation
    - e.g. change the lighting in an image
- Useful when you need more data
- Regularizes training by showing network more examples from manifold

Image Data

original

augmented

Text Data

I like doggos

I love doggos

I really love doggos

I really like doggos

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Upcoming Events

MIC Paper signup: https://goo.gl/iAm6TL
BUMIC Projects signup: https://goo.gl/GmP9oK

MIT MIC reading group:

Paper: Decoupled Neural Interfaces Using Synthetic Gradients
Location: MIT 56-154 (building 56, room 154)
Date: 10.12.17 Time: 5 PM

BU MIC reading group:

Paper: Self-Normalizing Neural Networks
Location: Fishbowl Conference Room
Date: 10.11.17 Time: 5 PM

Next workshop:

Topic: Compositional Data
Location: BU Hariri Seminar Room
Date: 10.17.17 Time: 7 PM

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References & Further Reading

[1] Fortmann-Roe, Scott. "Understanding the bias-variance tradeoff." (2012).

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[3] Ba, Jimmy, and Brendan Frey. "Adaptive dropout for training deep neural networks." *Advances in Neural Information Processing Systems*.2013.

[4] Zhang, Chiyuan, et al. "Understanding deep learning requires rethinking generalization." arXiv preprint arXiv:1611.03530 (2016).

[5] Krueger, David, et al. "Deep Nets Don't Learn via Memorization." (2017).

[6] Huang, Gao, et al. "Deep networks with stochastic depth." European Conference on Computer Vision. Springer International Publishing, 2016.

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[8] Krueger, David, et al. "Zoneout: Regularizing rnns by randomly preserving hidden activations." arXiv preprint arXiv:1606.01305 (2016).

[9] Sun, Xu, et al. "meProp: Sparsified Back Propagation for Accelerated Deep Learning with Reduced Overfitting." arXiv preprint arXiv:1706.06197 (2017).

[10] https://medium.com/towards-data-science/image-augmentation-for-deep-learning-histogram-equalization-a71387f609b2

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