Deep Learning for Computer Vision

Regularization in Neural Networks

Vineeth N Balasubramanian

Department of Computer Science and Engineering
Indian Institute of Technology, Hyderabad

Review

Questions

- How to know if you are in a local minima (or any other critical point on the loss surface)?

Review

Questions

- How to know if you are in a local minima (or any other critical point on the loss surface)? We will see this in this lecture
- Why is training deep neural networks using GD and Mean-Squared Error (MSE) as cost function, a non-convex optimization problem?

Review

Questions

- How to know if you are in a local minima (or any other critical point on the loss surface)? We will see this in this lecture
- Why is training deep neural networks using GD and Mean-Squared Error (MSE) as cost function, a non-convex optimization problem? Non-linear activation functions can make the problem non-convex
- Let us assume a linear deep neural network (only linear activation functions, $f(x) = x$). Would using GD and MSE still be a non-convex problem?

Review

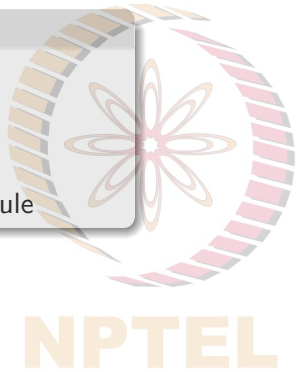
Questions

- How to know if you are in a local minima (or any other critical point on the loss surface)? We will see this in this lecture
- Why is training deep neural networks using GD and Mean-Squared Error (MSE) as cost function, a non-convex optimization problem? Non-linear activation functions can make the problem non-convex
- Let us assume a linear deep neural network (only linear activation functions, $f(x) = x$). Would using GD and MSE still be a non-convex problem? Yes! Weight symmetry is a reason

What is Regularization? An Intuitive View

What's my rule?

- 1 2 3 $\Longrightarrow$ satisfies rule
- 4 5 6 $\Longrightarrow$ satisfies rule
- 7 8 9 $\Longrightarrow$ satisfies rule
- 9 2 31 $\Longrightarrow$ does not satisfy rule



What is Regularization? An Intuitive View

What's my rule?

- 1 2 3 $\implies$ satisfies rule
- 4 5 6 $\implies$ satisfies rule
- 7 8 9 $\implies$ satisfies rule
- 9 2 31 $\implies$ does not satisfy rule

Plausible rules

- 3 consecutive single digits
- 3 consecutive integers
- 3 numbers in ascending order
- 3 numbers whose sum is less than 25
- 3 numbers < 10
- 1, 4, or 7 in first column
- "yes" to first 3 sequences, "no" to all others

What is Regularization? An Intuitive View

What's my rule?

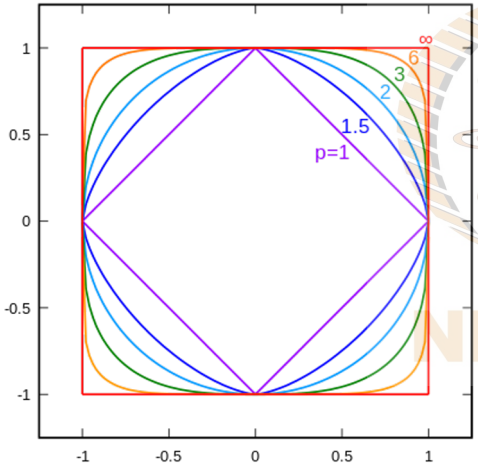
- 1 2 3 $\implies$ satisfies rule
- 4 5 6 $\implies$ satisfies rule
- 7 8 9 $\implies$ satisfies rule
- 9 2 31 $\implies$ does not satisfy rule

Plausible rules

- 3 consecutive single digits
- 3 consecutive integers
- 3 numbers in ascending order
- 3 numbers whose sum is less than 25
- 3 numbers < 10
- 1, 4, or 7 in first column
- "yes" to first 3 sequences, "no" to all others

Regularization corresponds to methods used in machine learning to improve **generalization performance** (avoid overfitting to training data)

Review: L_p Norms



- All p-norms penalize larger weights
- $p < 2$ tends to create sparse (i.e. lots of 0 weights)
- $p > 2$ tends to like similar weights

Credit: David Kauchak, Pomona Univ

L2 Regularization

- Penalty on L2-norm of parameters commonly known as L_2 **weight decay**, or simply **weight decay**
- Loss function defined by:

$$\widetilde{\mathcal{L}}(w) = \mathcal{L}(w) + \frac{\alpha}{2} \|w\|^2$$

Credit: Ali Ghodsi, University of Waterloo; Mitesh Khapra, IIT Madras

L2 Regularization

- Penalty on L2-norm of parameters commonly known as L_2 **weight decay**, or simply **weight decay**
- Loss function defined by:

$$\widetilde{\mathcal{L}}(w) = \mathcal{L}(w) + \frac{\alpha}{2} \|w\|^2$$

- Gradient of total objective function:

$$\nabla \widetilde{\mathcal{L}}(w) = \nabla \mathcal{L}(w) + \alpha w$$

Credit: Ali Ghodsi, University of Waterloo; Mitesh Khapra, IIT Madras

L2 Regularization

- Penalty on L2-norm of parameters commonly known as L_2 **weight decay**, or simply **weight decay**
- Loss function defined by:

$$\widetilde{\mathcal{L}}(w) = \mathcal{L}(w) + \frac{\alpha}{2} \|w\|^2$$

- Gradient of total objective function:

$$\nabla \widetilde{\mathcal{L}}(w) = \nabla \mathcal{L}(w) + \alpha w$$

- Update rule:

$$w_{t+1} = w_t - \eta \nabla \mathcal{L}(w_t) - \eta \alpha w_t$$

Credit: Ali Ghodsi, University of Waterloo; Mitesh Khapra, IIT Madras

L2 Regularization: Analysis

- Let w^* be optimal solution in absence of regularization [i.e. $\nabla \mathcal{L}(w^*) = 0$]

L2 Regularization: Analysis

- Let w^* be optimal solution in absence of regularization [i.e. $\nabla \mathcal{L}(w^*) = 0$]
- Consider $u = w - w^*$. Using Taylor series approximation upto 2^{nd} order:

$$\mathcal{L}(w^* + u) = \mathcal{L}(w^*) + u^T \nabla \mathcal{L}(w^*) + \frac{1}{2} u^T H u$$

L2 Regularization: Analysis

- Let w^* be optimal solution in absence of regularization [i.e. $\nabla \mathcal{L}(w^*) = 0$]
- Consider $u = w - w^*$. Using Taylor series approximation upto 2^{nd} order:

$$\mathcal{L}(w^* + u) = \mathcal{L}(w^*) + u^T \nabla \mathcal{L}(w^*) + \frac{1}{2} u^T H u$$

$$\begin{aligned} \mathcal{L}(w) &= \mathcal{L}(w^*) + (w - w^*)^T \nabla \mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \\ &= \mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \qquad (\because \nabla \mathcal{L}(w^*) = 0) \end{aligned} \tag{1}$$

L2 Regularization: Analysis

- Let w^* be optimal solution in absence of regularization [i.e. $\nabla \mathcal{L}(w^*) = 0$]
- Consider $u = w - w^*$. Using Taylor series approximation upto 2^{nd} order:

$$\mathcal{L}(w^* + u) = \mathcal{L}(w^*) + u^T \nabla \mathcal{L}(w^*) + \frac{1}{2} u^T H u$$

$$\begin{aligned} \mathcal{L}(w) &= \mathcal{L}(w^*) + (w - w^*)^T \nabla \mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \\ &= \mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \qquad (\because \nabla \mathcal{L}(w^*) = 0) \end{aligned} \tag{1}$$

- Taking derivative:

$$\nabla \mathcal{L}(w) = \nabla \mathcal{L}(w^*) + H(w - w^*) = H(w - w^*)$$

L2 Regularization: Analysis

- Let w^* be optimal solution in absence of regularization [i.e. $\nabla\mathcal{L}(w^*) = 0$]
- Consider $u = w - w^*$. Using Taylor series approximation upto 2^{nd} order:

$$\mathcal{L}(w^* + u) = \mathcal{L}(w^*) + u^T\nabla\mathcal{L}(w^*) + \frac{1}{2}u^T H u$$

$$\begin{aligned}\mathcal{L}(w) &= \mathcal{L}(w^*) + (w - w^*)^T\nabla\mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H(w - w^*) \\ &= \mathcal{L}(w^*) + \frac{1}{2}(w - w^*)^T H(w - w^*) \qquad (\because \nabla\mathcal{L}(w^*) = 0)\end{aligned} \tag{1}$$

- Taking derivative:

$$\nabla\mathcal{L}(w) = \nabla\mathcal{L}(w^*) + H(w - w^*) = H(w - w^*)$$

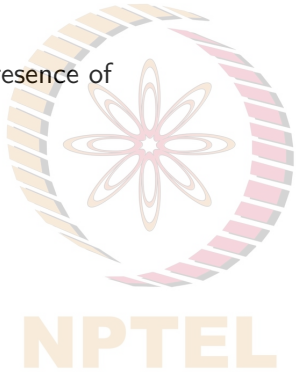
- Gradient of total objective function (in presence of L2 regularization):

$$\nabla\widetilde{\mathcal{L}}(w) = \nabla\mathcal{L}(w) + \alpha w = H(w - w^*) + \alpha w$$

Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

L2 Regularization: Analysis

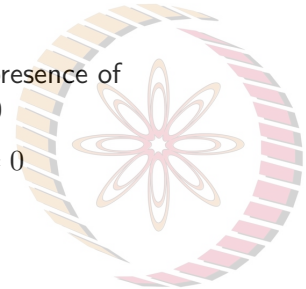
- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$



L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$



L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$

$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$

L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$

$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$

$$\implies \widetilde{w} = (H + \alpha\mathbb{I})^{-1}Hw^*$$

L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$

$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$

$$\implies \widetilde{w} = (H + \alpha\mathbb{I})^{-1}Hw^*$$

- If $\alpha \to 0$, then $\widetilde{w} \to w^*$; and therefore no regularization

L2 Regularization: Analysis

- What happens when $\alpha \neq 0$?

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla \widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha \widetilde{w} = 0$$

$$\therefore (H + \alpha \mathbb{I})\widetilde{w} = Hw^*$$

$$\implies \widetilde{w} = (H + \alpha \mathbb{I})^{-1} H w^*$$

- If $\alpha \to 0$, then $\widetilde{w} \to w^*$; and therefore no regularization

L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$

$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$

$$\implies \widetilde{w} = (H + \alpha\mathbb{I})^{-1}Hw^*$$

- If $\alpha \to 0$, then $\widetilde{w} \to w^*$; and therefore no regularization

- What happens when $\alpha \neq 0$? If H is symmetric positive semidefinite, $H = Q\Lambda Q^T$, where Q is orthogonal i.e. $QQ^T = Q^TQ = \mathbb{I}$

L2 Regularization: Analysis

- Let $\widetilde{w}$ be optimal solution in presence of regularization, i.e. $\nabla\widetilde{\mathcal{L}}(\widetilde{w}) = 0$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$

$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$

$$\implies \widetilde{w} = (H + \alpha\mathbb{I})^{-1}Hw^*$$

- If $\alpha \to 0$, then $\widetilde{w} \to w^*$; and therefore no regularization

- What happens when $\alpha \neq 0$? If H is symmetric positive semidefinite, $H = Q\Lambda Q^T$, where Q is orthogonal i.e. $QQ^T = Q^TQ = \mathbb{I}$

$$\begin{aligned}
\widetilde{w} &= (H + \alpha\mathbb{I})^{-1}Hw^* \\
&= (Q\Lambda Q^T + \alpha\mathbb{I})^{-1}Q\Lambda Q^Tw^* \\
&= (Q\Lambda Q^T + \alpha Q\mathbb{I}Q^T)^{-1}Q\Lambda Q^Tw^* \\
&= [Q(\Lambda + \alpha\mathbb{I})Q^T]^{-1}Q\Lambda Q^Tw^* \\
&= Q^{T^{-1}}(\Lambda + \alpha\mathbb{I})^{-1}Q^{-1}Q\Lambda Q^Tw^* \\
&= Q(\Lambda + \alpha\mathbb{I})^{-1}\Lambda Q^Tw^* (\because Q^{T^{-1}} = Q)
\end{aligned}$$

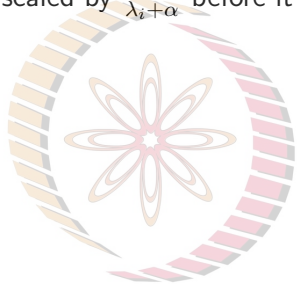
Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

L2 Regularization: Analysis

- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i + \alpha}$ before it is rotated back by Q

L2 Regularization: Analysis

- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by Q
- If $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$



L2 Regularization: Analysis

- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by Q
- If $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$
- If $\lambda_i << \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 0$

L2 Regularization: Analysis

- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by Q
- If $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$
- If $\lambda_i << \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 0$
- Thus, only significant directions (larger eigenvalues) will be retained.

$$\text{Effective parameters} = \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_i + \alpha} < n$$

L2 Regularization: Analysis

- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by Q
- If $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$
- If $\lambda_i << \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 0$
- Thus, only significant directions (larger eigenvalues) will be retained.

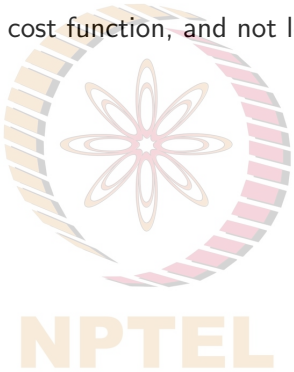
$$\text{Effective parameters} = \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_i + \alpha} < n$$

- Summary: The weight vector (w^*) is getting rotated to $\widetilde{w}$ on using L2 regularization. All of its elements are shrinking but some are shrinking more than the others. This ensures that only important features are given high weights.

Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

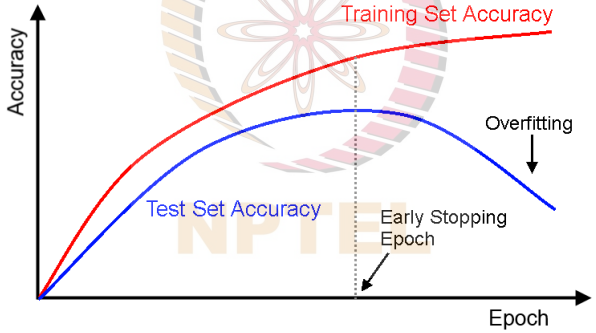
Early Stopping

- **Simple idea:** keep monitoring cost function, and not let it become too low consistently; stop at an earlier iteration



Early Stopping

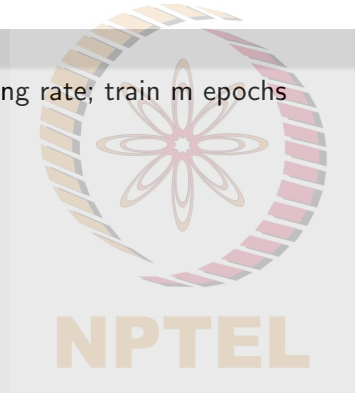
- **Simple idea:** keep monitoring cost function, and not let it become too low consistently; stop at an earlier iteration



Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs



Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach

Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach
- **Error-change criterion:**
  - Stop when error isn't dropping over a window of, say, 10 epochs

Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach
- **Error-change criterion:**
  - Stop when error isn't dropping over a window of, say, 10 epochs
  - Train for a fixed number of epochs after criterion is reached (possibly with lower learning rate)

Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach
- **Error-change criterion:**
  - Stop when error isn't dropping over a window of, say, 10 epochs
  - Train for a fixed number of epochs after criterion is reached (possibly with lower learning rate)
- **Weight-change criterion:**
  - Compare weights at epochs $t - 10$ and t and test: $\max_i \|w_i^t - w_i^{t-10}\| < \rho$

Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach
- **Error-change criterion:**
  - Stop when error isn't dropping over a window of, say, 10 epochs
  - Train for a fixed number of epochs after criterion is reached (possibly with lower learning rate)
- **Weight-change criterion:**
  - Compare weights at epochs $t - 10$ and t and test: $\max_i \|w_i^t - w_i^{t-10}\| < \rho$
  - Don't base on length of overall weight change vector

Early Stopping

When to stop?

- Train n epochs; lower learning rate; train m epochs $\rightarrow$ Bad idea: can't assume one-size-fits-all approach
- **Error-change criterion:**
  - Stop when error isn't dropping over a window of, say, 10 epochs
  - Train for a fixed number of epochs after criterion is reached (possibly with lower learning rate)
- **Weight-change criterion:**
  - Compare weights at epochs $t - 10$ and t and test: $\max_i \|w_i^t - w_i^{t-10}\| < \rho$
  - Don't base on length of overall weight change vector
  - Possibly express as a percentage of the weight

Dataset Augmentation

- Creation of data using some knowledge of task

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations
  - Color changes

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations
  - Color changes
  - Noise injection

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations
  - Color changes
  - Noise injection
  - Mirroring

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations
  - Color changes
  - Noise injection
  - Mirroring
- Helps increase data; is useful when training data provided is less (DNNs need large amounts of training data to work!)

Dataset Augmentation

- Creation of data using some knowledge of task
- Exploit the fact that certain transformations to image do not change label of image
- Methods:
  - Data jittering (E.g. Distortion and blurring of images)
  - Rotations
  - Color changes
  - Noise injection
  - Mirroring
- Helps increase data; is useful when training data provided is less (DNNs need large amounts of training data to work!)
- Also acts as regularizer (by avoiding overfitting to provided data)

Dataset Augmentation: Example[1]

[1] Wu, Ren, et al. "Deep image: Scaling up image recognition." arXiv 2015

Dataset Augmentation: Example[1]

[1]Wu, Ren, et al. "Deep image: Scaling up image recognition." arXiv 2015

Data Augmentation: Newer Methods

Mixup

- Create virtual training examples as below ($\lambda \in [0, 1]$):

$$\tilde{x} = \lambda x_i + (1 - \lambda) x_j$$

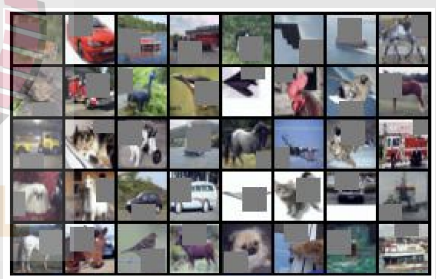
$$\tilde{y} = \lambda y_i + (1 - \lambda) y_j$$

where x_i,x_j are input vectors, and y_i,y_j are one-hot label encodings

- *Variants:* Manifold Mixup, AugMix

CutOut

- Randomly mask out square regions of input during training



- *Variants:* CutMix

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**
  - Addd noise to data while training

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**
  - Addd noise to data while training
  - Adding Gaussian noise to input is equivalent to weight decay (L_2 regularisation) when loss function is sum-of-squared error[2]. Homework!

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**
  - Addd noise to data while training
  - Adding Gaussian noise to input is equivalent to weight decay (L_2 regularisation) when loss function is sum-of-squared error[2]. Homework!
  - Can be interpreted as form of **dataset augmentation.**

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**
  - Addd noise to data while training
  - Adding Gaussian noise to input is equivalent to weight decay (L_2 regularisation) when loss function is sum-of-squared error[2]. Homework!
  - Can be interpreted as form of **dataset augmentation.**
- **Label Noise**

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Noise Injection

Injecting noise is another form of regularization; has shown impressive results in certain applications:

- **Data Noise**
  - Addd noise to data while training
  - Adding Gaussian noise to input is equivalent to weight decay (L_2 regularisation) when loss function is sum-of-squared error[2]. Homework!
  - Can be interpreted as form of **dataset augmentation.**
- **Label Noise**
- **Gradient Noise**

[2] Bishop. Training with noise is equivalent to Tikhonov regularization. Neural Computation, 1995

Regularization through Label Noise[3]

- Disturb each training sample with probability α.
- For each disturbed sample, label randomly drawn from uniform distribution over $\{1, 2, \cdots, C\}$, regardless of true label

Algorithm 1 DisturbLabel

Input: $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^{N}$, noise rate α.
Initialization: a network model $\mathbb{M}$: $\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}_0) \in \mathbb{R}^C$;
for each mini-batch $\mathcal{D}_t = \{(\mathbf{x}_m, \mathbf{y}_m)\}_{m=1}^{M}$ **do**
  for each sample $(\mathbf{x}_m, \mathbf{y}_m)$ **do**
    Generate a disturbed label $\widetilde{\mathbf{y}}_m$ with Eqn (2);
  end for
  Update the parameters $\boldsymbol{\theta}_t$ with Eqn (1);
end for
Output: the trained model $\mathbb{M}'$: $\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}_T) \in \mathbb{R}^C$.

$$\begin{cases} \widetilde{c} & \sim & \mathcal{P}(\alpha), \\ \widetilde{y}_{\widetilde{c}} & = & 1, \\ \widetilde{y}_i & = & 0, \qquad \forall i \neq \widetilde{c}. \end{cases} \tag{2}$$

[3] Xie, Lingxi, et al. "DisturbLabel: Regularizing CNN on the Loss Layer." CVPR 2016.

Regularization through Gradient Noise[4]

- **Idea:** Add noise to gradient

$$g_t \leftarrow g_t + N(0, \sigma_t^2)$$

[4] Neelakantan, Arvind, et al. "Adding gradient noise improves learning for very deep networks." arXiv preprint arXiv:1511.06807 (2015)

Regularization through Gradient Noise[4]

- **Idea:** Add noise to gradient

$$g_t \leftarrow g_t + N(0, \sigma_t^2)$$

- Annealed Gaussian noise by decaying variance

$$\sigma_t^2 = \frac{\eta}{(1+t)^\gamma}$$

[4] Neelakantan, Arvind, et al. "Adding gradient noise improves learning for very deep networks." arXiv preprint arXiv:1511.06807 (2015)

Regularization through Gradient Noise[4]

- **Idea:** Add noise to gradient

$$g_t \leftarrow g_t + N(0, \sigma_t^2)$$

- Annealed Gaussian noise by decaying variance

$$\sigma_t^2 = \frac{\eta}{(1+t)^\gamma}$$

- Showed significant improvement in performance in certain applications

[4] Neelakantan, Arvind, et al. "Adding gradient noise improves learning for very deep networks." arXiv preprint arXiv:1511.06807 (2015)

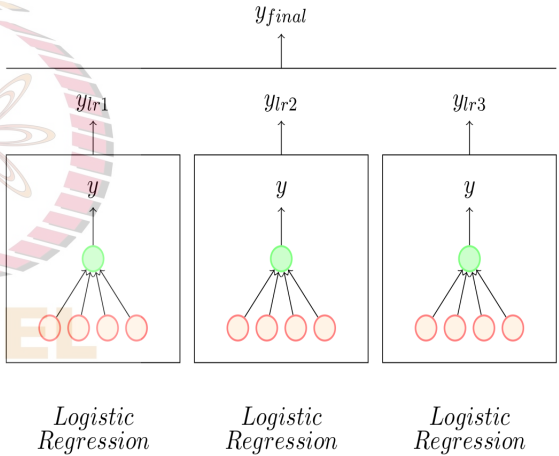
Ensemble Methods

- Train several different models separately, then have all models vote on the output for test examples
- An example of a general strategy in machine learning called **model averaging**
- Models can correspond to different classifiers, or could be different instances of same classifier trained with:
  - different hyperparameters
  - different features
  - different samples of the training data

Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

Ensemble Methods

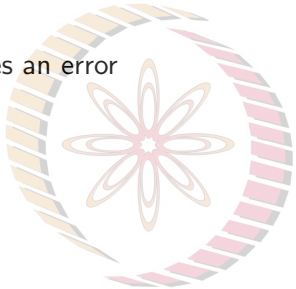
- **Bagging** (short for bootstrap aggregating): reduces generalization error by forming an ensemble using different instances of same classifier
- For e.g., consider a set of k logistic regression models
- Given a dataset, construct multiple training sets by sampling with replacement $(T_1, T_2, ..., T_k)$
- Train i^{th} instance of classifier using training set T_i



Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

Ensemble Methods

- Suppose that each model makes an error ε_i on a test example



Ensemble Methods

- Suppose that each model makes an error ε_i on a test example
- Let ε_i be drawn from a zero-mean multivariate normal distribution with:

$$\text{Variance} = \mathbb{E}[\varepsilon_i^2] = V$$
$$\text{Covariance} = \mathbb{E}[\varepsilon_i \varepsilon_j] = C$$

Ensemble Methods

- Suppose that each model makes an error ε_i on a test example
- Let ε_i be drawn from a zero-mean multivariate normal distribution with:

$$\text{Variance} = \mathbb{E}[\varepsilon_i^2] = V$$
$$\text{Covariance} = \mathbb{E}[\varepsilon_i \varepsilon_j] = C$$

- Error made by average prediction of all models is $\frac{1}{k}\sum_i \varepsilon_i$

Ensemble Methods

- Suppose that each model makes an error ε_i on a test example
- Let ε_i be drawn from a zero-mean multivariate normal distribution with:

$$\text{Variance} = \mathbb{E}[\varepsilon_i^2] = V$$
$$\text{Covariance} = \mathbb{E}[\varepsilon_i \varepsilon_j] = C$$

- Error made by average prediction of all models is $\frac{1}{k}\sum_i \varepsilon_i$

Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

- Expected squared error of ensemble predictor is:

$$\begin{aligned} MSE &= \mathbb{E}\left[\left(\frac{1}{k}\sum_i \varepsilon_i\right)^2\right] \\ &= \frac{1}{k^2}\mathbb{E}\left[\sum_i \sum_{j=i} \varepsilon_i \varepsilon_j + \sum_i \sum_{j \neq i} \varepsilon_i \varepsilon_j\right] \\ &= \frac{1}{k^2}\mathbb{E}\left[\sum_i \varepsilon_i^2 + \sum_i \sum_{j \neq i} \varepsilon_i \varepsilon_j\right] \\ &= \frac{1}{k^2}(kV + k(k-1)C) \\ &= \frac{1}{k}V + \frac{k-1}{k}C \end{aligned}$$

Ensemble Methods

- Expected squared error of ensemble predictor:

$$MSE = \frac{1}{k}V + \frac{k-1}{k}C$$

What does this tell you?

Ensemble Methods

- Expected squared error of ensemble predictor:

$$MSE = \frac{1}{k}V + \frac{k-1}{k}C$$

What does this tell you?

- If errors of model are perfectly correlated, then $V = C$ and $MSE = V$, i.e. bagging does not help: the MSE of ensemble is as bad as individual models

Ensemble Methods

- Expected squared error of ensemble predictor:

$$MSE = \frac{1}{k}V + \frac{k-1}{k}C$$

What does this tell you?

- If errors of model are perfectly correlated, then $V = C$ and $MSE = V$, i.e. bagging does not help: the MSE of ensemble is as bad as individual models
- If errors of model are independent or uncorrelated, then $C = 0$ and MSE of ensemble reduces to $\frac{1}{k}V$
- On average, **ensemble will perform at least as well as its individual members**

Credit: Ali Ghodsi, Univ of Waterloo; Mitesh Khapra, IIT Madras

Dropout

- One major issue in learning large neural networks is **co-adaptation**
  - As network is trained iteratively, powerful connections are learned more while weaker ones are ignored
  - After many iterations, only a fraction of node connections participate
  - Therefore, expanding neural network size may not help

Dropout

- One major issue in learning large neural networks is **co-adaptation**
  - As network is trained iteratively, powerful connections are learned more while weaker ones are ignored
  - After many iterations, only a fraction of node connections participate
  - Therefore, expanding neural network size may not help
- **Dropout**: Regularization method to address this issue

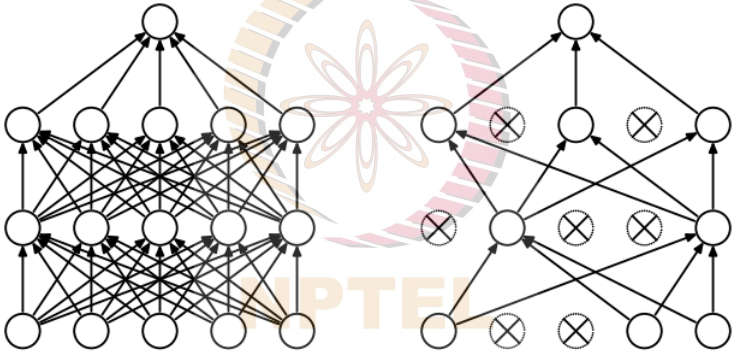
Dropout

- One major issue in learning large neural networks is **co-adaptation**
  - As network is trained iteratively, powerful connections are learned more while weaker ones are ignored
  - After many iterations, only a fraction of node connections participate
  - Therefore, expanding neural network size may not help
- **Dropout**: Regularization method to address this issue
- **Training Phase:** For each hidden layer, for each training sample, for each iteration, ignore (zero out) a random fraction, p, of nodes (and corresponding activations)

Dropout

- One major issue in learning large neural networks is **co-adaptation**
  - As network is trained iteratively, powerful connections are learned more while weaker ones are ignored
  - After many iterations, only a fraction of node connections participate
  - Therefore, expanding neural network size may not help
- **Dropout**: Regularization method to address this issue
- **Training Phase:** For each hidden layer, for each training sample, for each iteration, ignore (zero out) a random fraction, p, of nodes (and corresponding activations)
- **Test Phase:** Use all activations, but reduce them by factor p (to account for missing activations during training)

Dropout



(a) Standard Neural Net (b) After applying dropout. [5]

[5] Srivastava, Nitish, et al. "Dropout: a simple way to prevent neural networks from overfitting", JMLR 2014

Dropout

- Recall ensemble methods: with H hidden units, each of which can be dropped, we can have 2^H possible models

Dropout

- Recall ensemble methods: with H hidden units, each of which can be dropped, we can have 2^H possible models
- This is prohibitively large and we cannot possibly train so many networks

Dropout

- Recall ensemble methods: with H hidden units, each of which can be dropped, we can have 2^H possible models
- This is prohibitively large and we cannot possibly train so many networks
- Trick: Each of the 2^{H-1} models that includes hidden unit h must share the same weight for the unit
  - serves as a form of regularization
  - makes the models cooperate

Dropout

- Recall ensemble methods: with H hidden units, each of which can be dropped, we can have 2^H possible models
- This is prohibitively large and we cannot possibly train so many networks
- Trick: Each of the 2^{H-1} models that includes hidden unit h must share the same weight for the unit
  - serves as a form of regularization
  - makes the models cooperate
- Including all hidden units at test time with scaling of $\frac{1}{2}$ is equivalent to computing geometric mean of all 2^H models.

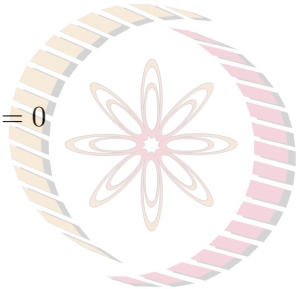
Dropout

- Recall ensemble methods: with H hidden units, each of which can be dropped, we can have 2^H possible models
- This is prohibitively large and we cannot possibly train so many networks
- Trick: Each of the 2^{H-1} models that includes hidden unit h must share the same weight for the unit
  - serves as a form of regularization
  - makes the models cooperate
- Including all hidden units at test time with scaling of $\frac{1}{2}$ is equivalent to computing geometric mean of all 2^H models. (How?)

Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

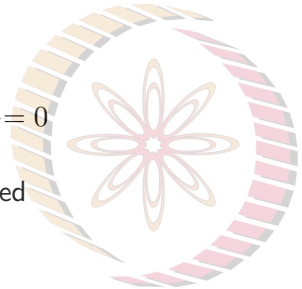


Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

- 2^n possible sub-networks indexed by k

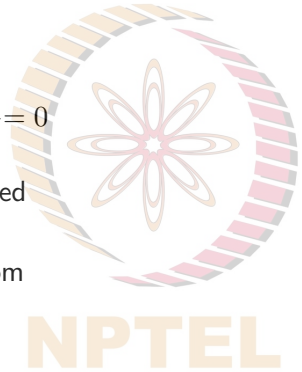


Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

- 2^n possible sub-networks indexed by k
- Geometric mean of outputs from all sub-networks: $G = \prod_k o_k^{\frac{1}{2^n}}$



Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

- 2^n possible sub-networks indexed by k
- Geometric mean of outputs from all sub-networks: $G = \prod_k o_k^{\frac{1}{2^n}}$
- Geometric mean of complementary outputs: $G' = \prod_k (1 - o_k)^{\frac{1}{2^n}}$

Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

- 2^n possible sub-networks indexed by k
- Geometric mean of outputs from all sub-networks: $G = \prod_k o_k^{\frac{1}{2^n}}$
- Geometric mean of complementary outputs: $G' = \prod_k (1 - o_k)^{\frac{1}{2^n}}$

- Normalized geometric mean $NGM = \frac{G}{G+G'}$.

Hence:

$$NGM = \frac{1}{1 + \left(\prod_k \frac{1-\sigma(x_k)}{\sigma(x_k)}\right)^{\frac{1}{2^n}}}$$

$$= \frac{1}{1 + \left(\prod_k ce^{-\lambda x_k}\right)^{\frac{1}{2^n}}} \left(\because \frac{1-\sigma(x)}{\sigma(x)} = ce^{-\lambda x} \right)$$

$$= \frac{1}{1 + c[e^{-\lambda \sum_k x_k/2^n}]} = \sigma(\mathbb{E}[x])$$

where $\mathbb{E}[x] = \sum_k x_k/2^n$

Dropout for Single Non-Linear Unit

- Consider a logistic sigmoidal function on input x:

$$o = \sigma(x) = \frac{1}{1 + ce^{-\lambda x}} \qquad c >= 0$$

- 2^n possible sub-networks indexed by k
- Geometric mean of outputs from all sub-networks: $G = \prod_k o_k^{\frac{1}{2^n}}$
- Geometric mean of complementary outputs: $G' = \prod_k (1 - o_k)^{\frac{1}{2^n}}$

- Normalized geometric mean $NGM = \frac{G}{G+G'}$.

Hence:

$$NGM = \frac{1}{1 + \left(\prod_k \frac{1-\sigma(x_k)}{\sigma(x_k)}\right)^{\frac{1}{2^n}}}$$

$$= \frac{1}{1 + \left(\prod_k ce^{-\lambda x_k}\right)^{\frac{1}{2^n}}} \left(\because \frac{1 - \sigma(x)}{\sigma(x)} = ce^{-\lambda x} \right)$$

$$= \frac{1}{1 + c[e^{-\lambda \sum_k x_k/2^n}]} = \sigma(\mathbb{E}[x])$$

where $\mathbb{E}[x] = \sum_k x_k/2^n$

NGM is equivalent to output of overall network with weights divided by two

Homework

Readings

- Deep Learning book, Chapter 7, Sections 7.1-7.5, 7.8, 7.12
- Tutorial on Dropout for more information (Optional)

Exercise

- Show that adding Gaussian noise (with zero mean) to input is equivalent to L_2 weight decay when loss function is MSE.

References I

[1] Geoffrey E. Hinton et al. "Improving neural networks by preventing co-adaptation of feature detectors". In: *CoRR* abs/1207.0580 (2012). arXiv: 1207.0580.

[2] Pierre Baldi and Peter Sadowski. "The dropout learning algorithm". In: *Artificial intelligence* 210 (2014), pp. 78–122.

[3] Nitish Srivastava et al. "Dropout: A Simple Way to Prevent Neural Networks from Overfitting". In: *Journal of Machine Learning Research* 15.56 (2014), pp. 1929–1958.

[4] David Warde-Farley et al. "An empirical analysis of dropout in piecewise linear networks". In: *CoRR* abs/1312.6197 (2014).

[5] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. MIT Press, 2016.

[6] Terrance DeVries and Graham W Taylor. "Improved Regularization of Convolutional Neural Networks with Cutout". In: *arXiv preprint arXiv:1708.04552* (2017).

[7] Hongyi Zhang et al. "mixup: Beyond Empirical Risk Minimization". In: *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings*. 2018.

References II

[8] *Ghodsi, Ali, STAT 946 - Deep Learning (Fall 2015)*. URL: https://uwaterloo.ca/data-analytics/sites/ca.data-analytics/files/uploads/files/f15_stat946_deep_learning_outline_1.pdf (visited on 06/05/2020).

[9] *Khapra, Mitesh M., CS 7015 - Deep Learning (Spring 2019)*. URL: https://www.cse.iitm.ac.in/~miteshk/CS7015.html (visited on 06/03/2020).