Neural Networks: Optimization & Regularization

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Machine Learning

Outline

1. **Optimization**
   - Momentum & Nesterov Momentum
   - AdaGrad & RMSProp
   - Continuation Methods & Curriculum Learning
   - Cyclic Learning Rates
   - NTK-based Initialization*
   - Batch Normalization
2. **Regularization**
   - Weight Decay
   - Data Augmentation
   - Self-Supervised Pre-training
   - Dropout
   - Manifold Regularization
   - More Domain-Specific Models

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Challenges

- NN a complex function:

$$\begin{aligned}\hat{\boldsymbol{y}} &= f(\boldsymbol{x};\Theta) \\ &= f^{(L)}(\cdots f^{(1)}(\boldsymbol{x};\boldsymbol{W}^{(1)});\boldsymbol{W}^{(L)})\end{aligned}$$

- Given a training set $\mathbb{X}$, our goal is to solve:

$$\begin{aligned}\arg\min_{\Theta} C(\Theta) &= \arg\min_{\Theta} -\log \mathrm{P}(\mathbb{X}\,|\,\Theta) \\ &= \arg\min_{\Theta} \sum_i -\log \mathrm{P}(\boldsymbol{y}^{(i)}\,|\,\boldsymbol{x}^{(i)},\Theta) \\ &= \arg\min_{\Theta} \sum_i C^{(i)}(\Theta) \\ &= \arg\min_{\boldsymbol{W}^{(1)},\cdots,\boldsymbol{W}^{(L)}} \sum_i C^{(i)}(\boldsymbol{W}^{(1)},\cdots,\boldsymbol{W}^{(L)})\end{aligned}$$

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- What are the challenges of solving this problem with SGD?

Training 101

- Before training a feedforward NN, remember to ***standardize*** (z-normalize) the input
  - Prevents dominating features
  - Improves conditioning

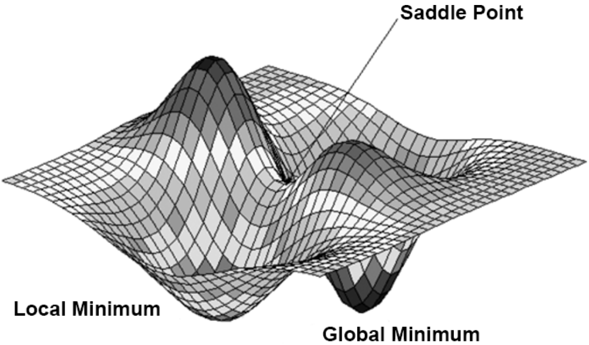
Training 101

- Before training a feedforward NN, remember to ***standardize*** (z-normalize) the input
  - Prevents dominating features
  - Improves conditioning
- When training, remember to:

1. Initialize all weights to small ***random values***
   - Breaks "symmetry" between different units so they are not updated in the same way
   - Biases $b^{(k)}$'s may be initialized to zero (or to small positive values for ReLUs to prevent too much saturation)
2. ***Early stop*** if the validation error does not continue decreasing
   - Prevents overfitting

Non-Convexity

- The loss function $C^{(i)}$ is ***non-convex***



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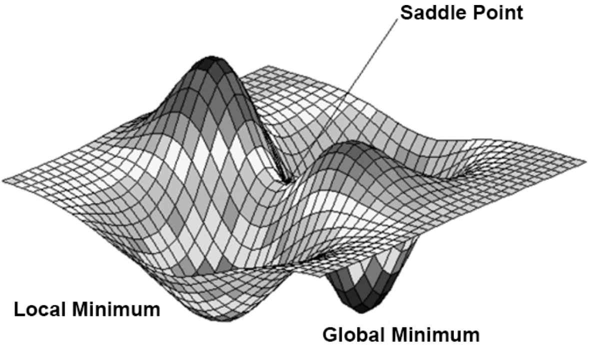

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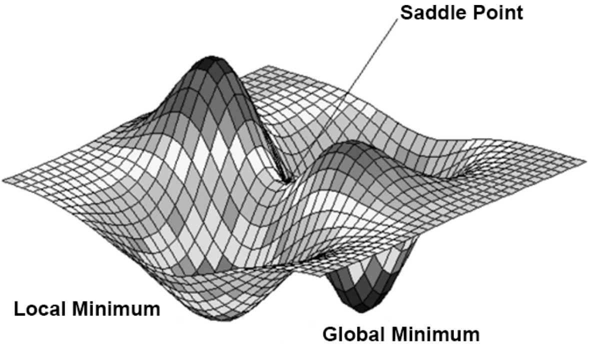

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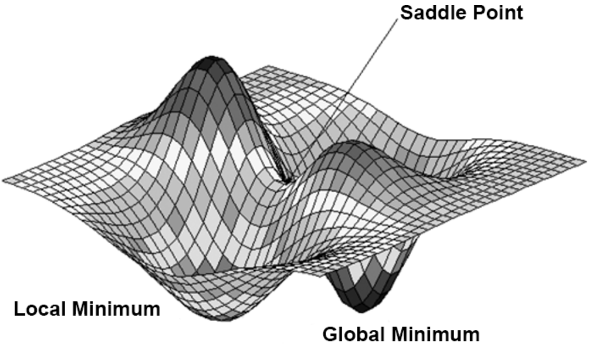

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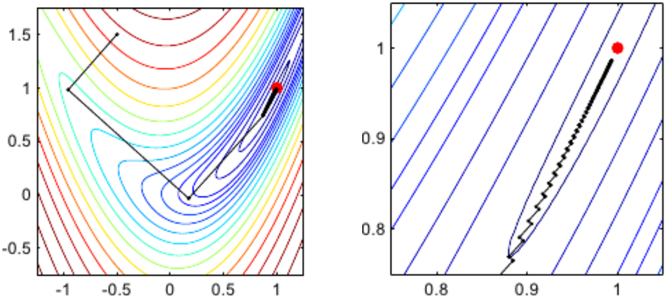
- However, studies [2, 4] show SGD seldom encounters critical points when training a large NN

Ill-Conditioning

- The loss $C^{(i)}$ may be ill-conditioned (in terms of Θ)
  - Due to, e.g., dependency between $W^{(k)}$'s at different layers



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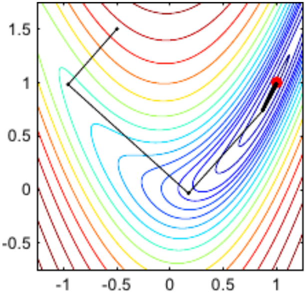

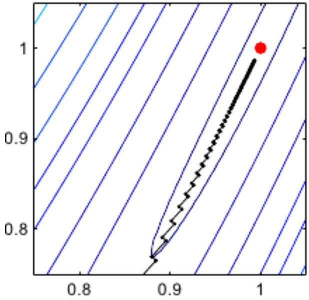

- SGD has slow progress at valleys or plateaus

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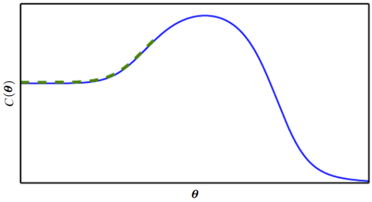
- SGD may proceed along a direction forever
- ***Initialization*** is important



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Momentum

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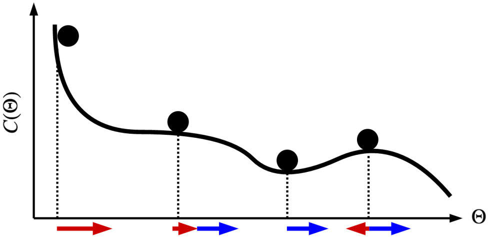
$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \eta \boldsymbol{g}^{(t)}$$

where $\boldsymbol{g}^{(t)} = \nabla_{\Theta} C(\Theta^{(t)})$



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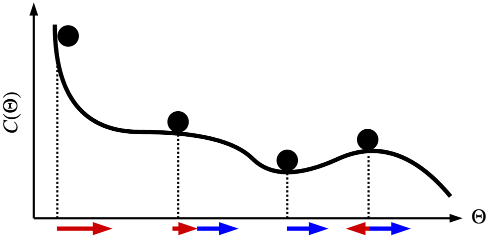

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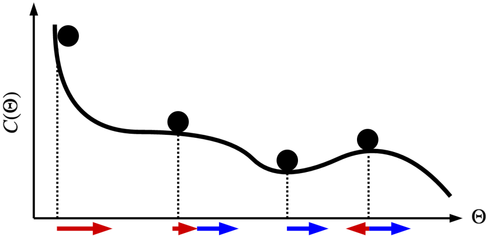

- Momentum: make the same movement $\boldsymbol{v}^{(t)}$ in the last iteration, corrected by negative gradient:

$$\boldsymbol{v}^{(t+1)} \leftarrow \lambda \boldsymbol{v}^{(t)} - (1-\lambda)\boldsymbol{g}^{(t)}$$

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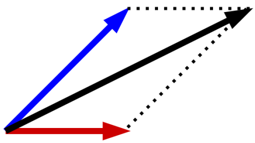

- $\boldsymbol{v}^{(t)}$ is a moving average of $-\boldsymbol{g}^{(t)}$

Nesterov Momentum

- Make the same movement $\boldsymbol{v}^{(t)}$ in the last iteration, corrected by ***lookahead*** negative gradient:

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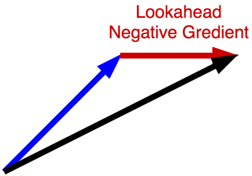

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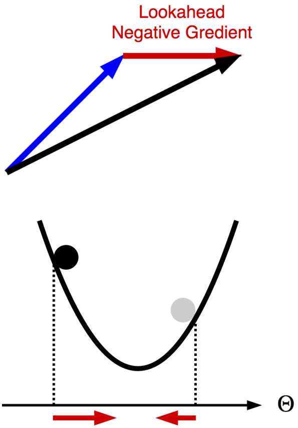

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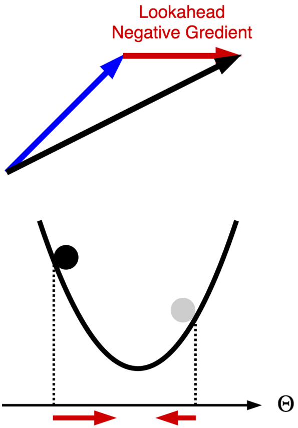
- Faster convergence to a minimum
- Not helpful for NNs that lack of minima



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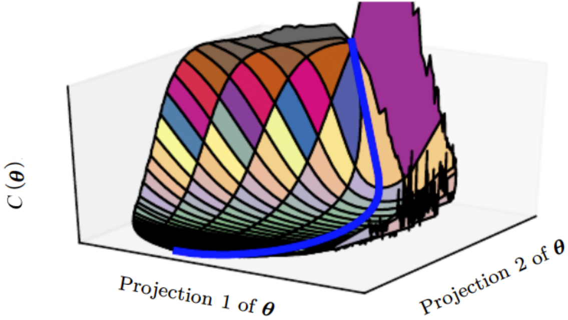
Where Does SGD Spend Its Training Time?



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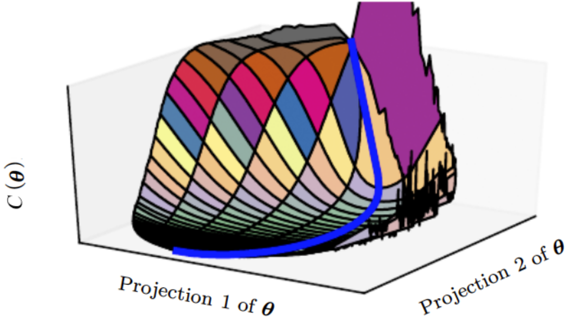
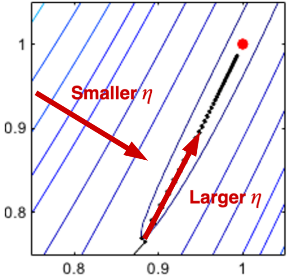


1. Detouring a saddle point of high cost
   - Better initialization
2. Traversing the relatively flat valley
   - Adaptive learning rate

SGD with Adaptive Learning Rates



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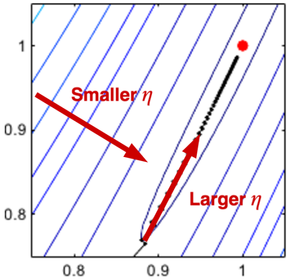

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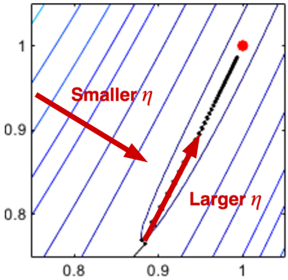

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- How?

AdaGrad

- Update rule:

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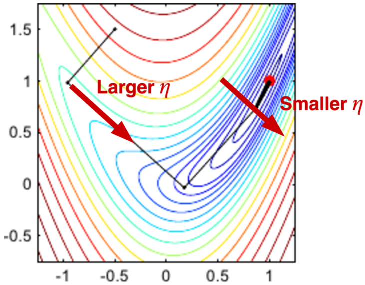
1. ***Smaller learning rate along all directions as t grows***
2. ***Larger learning rate along more gently sloped directions***

Limitations



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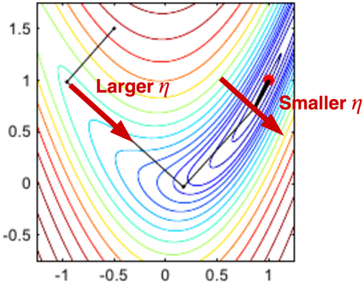

- The optimal learning rate along a direction may ***change over time***
- In AdaGrad, $\boldsymbol{r}^{(t+1)}$ accumulates squared gradients ***from the beginning of training***
  - Results in premature adaptivity

RMSProp

- ***RMSProp*** changes the gradient accumulation in $\boldsymbol{r}^{(t+1)}$ into a moving average:

$$\boldsymbol{r}^{(t+1)} \leftarrow \lambda \boldsymbol{r}^{(t)} + (1-\lambda)\boldsymbol{g}^{(t)} \odot \boldsymbol{g}^{(t)}$$

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- A popular algorithm ***Adam*** (short for ***adaptive moments***) [7] is a combination of RMSProp and Momentum:

$$\boldsymbol{v}^{(t+1)} \leftarrow \lambda_1 \boldsymbol{v}^{(t)} - (1-\lambda_1)\boldsymbol{g}^{(t)}$$

$$\boldsymbol{r}^{(t+1)} \leftarrow \lambda_2 \boldsymbol{r}^{(t)} + (1-\lambda_2)\boldsymbol{g}^{(t)} \odot \boldsymbol{g}^{(t)}$$

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  - With some bias corrections for $\boldsymbol{v}^{(t+1)}$ and $\boldsymbol{r}^{(t+1)}$

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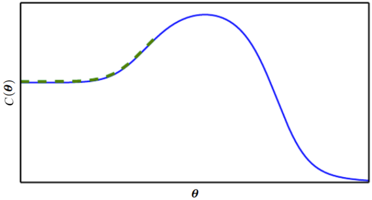
- *Initialization* is important



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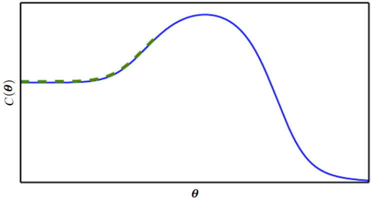


- How to better initialize $\Theta^{(0)}$?

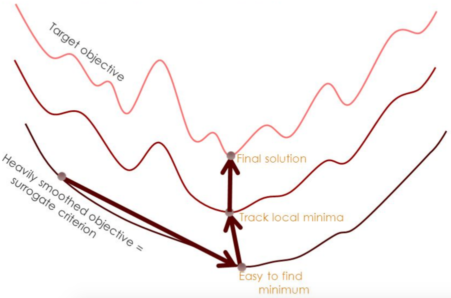
1. Train an NN multiple times with random initial points, and then pick the best
   - Slow
2. Design a series of cost functions such that a solution to one is a good initial point of the next
   - Solve the "easy" problem first, and then a "harder" one, and so on
3. Calculate initial gradients carefully
4. NTK-based initialization

Continuation Methods I

- ***Continuation methods***: construct easier cost functions by ***smoothing*** the original cost function:

$$\tilde{C}(\Theta) = \mathrm{E}_{\tilde{\Theta} \sim \mathcal{N}(\Theta, \sigma^2)} C(\tilde{\Theta})$$

  - In practice, we sample several $\tilde{\Theta}$'s to approximate the expectation
- Assumption: some non-convex functions become approximately convex when smoothen



Continuation Methods II

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- Designed to deal with local minima; not very helpful for NNs without minima

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- ***Curriculum learning*** (or ***shaping***) [1]: make the cost function easier by increasing the influence of ***simpler examples***
  - E.g., by assigning them larger weights in the new cost function
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- Learn simple concepts first, then learn more complex concepts that depend on these simpler concepts
  - Just like how humans learn
  - Knowing the principles, we are less likely to explain an observation using special (but wrong) rules

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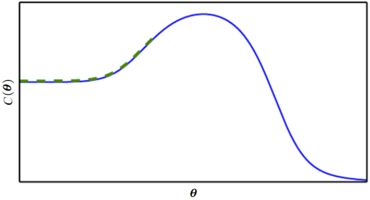
SGD Gradients are Noisy

- ***Initialization*** is important
- SGD gradients may not be representative in the beginning (and in the end)



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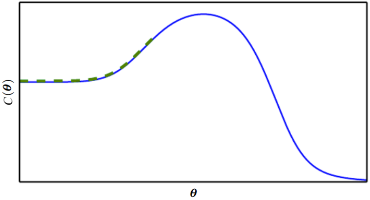
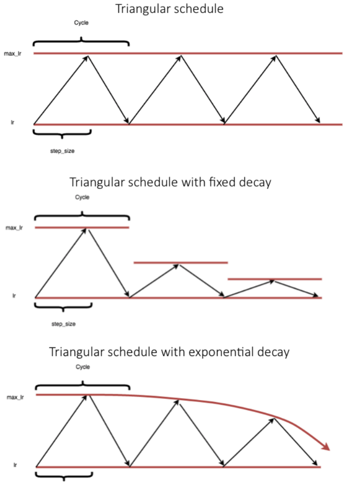


- Use a small learning rate in the very beginning [10]



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Prior Predictions of NTK-GP

- Prior (unconditioned) mean predictions for training set:

$$\hat{\boldsymbol{y}}_N = (\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}_N$$

- Prior mean predictions for test set:

$$\hat{\boldsymbol{y}}_M = \boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}(\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}_N$$

- Given a training set, the $\boldsymbol{T}_{N,N}$ and $\boldsymbol{T}_{M,N}$ depends only on the network structure and hyperparameters of initial weights

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- Let $\boldsymbol{T}_{N,N} = \boldsymbol{U}^\top \begin{bmatrix} \lambda_{\max} & & \\ & \ddots & \\ & & \lambda_{\min} \end{bmatrix} \boldsymbol{U}$, we have

$$(\boldsymbol{U}\hat{\boldsymbol{y}}_N)_i \approx ((\boldsymbol{I} - e^{-2\frac{\lambda_i}{\lambda_{\max}}t})\boldsymbol{U}\boldsymbol{y}_N)_i$$

- It follows that if ***the conditioning number $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$ diverges***, the NN becomes untrainable

Generalization

- Prior mean predictions for test set: $\hat{\boldsymbol{y}}_M = \boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}(\boldsymbol{I} - e^{-\eta \boldsymbol{T}_{N,N} t})\boldsymbol{y}_N$
- As $t \to \infty$ (trained), we have

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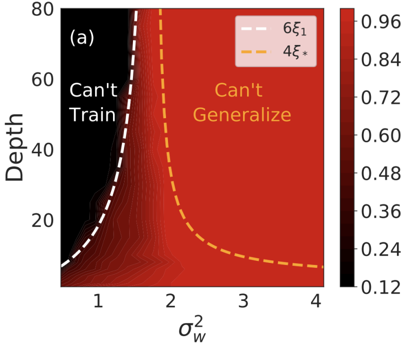
- If $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}$ ***is a data-independent constant matrix***, then the NN will fail to generalize
  - Constant rows $\Rightarrow$ independent with $\mathbb{X}$
  - Constant columns $\Rightarrow$ independent with $\boldsymbol{X}_M$
  - If $\boldsymbol{y}_N$ has zero mean, this implies that $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}\boldsymbol{y}_N = \boldsymbol{0}$

Results

- The training and test accuracy (color) of a fully-connected NN trained with SGD
  - (a) The NN is untrainable because κ is too large
  - (b) The NN is ungeneralizable because $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}\boldsymbol{y}_N$ is too small



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- What are the difficulties in training a deep NN?

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- The curvature of f with respect to any two $w^{(i)}$ and $w^{(j)}$ is

$$\frac{\partial f}{\partial w^{(i)} \partial w^{(j)}} = (w^{(i)} + w^{(j)}) \cdot x \prod_{k \neq i,j} w^{(k)}$$

  - Very small if L is large and $w^{(k)} < 1$ for $k \neq i,j$
  - Very large if L is large and $w^{(k)} > 1$ for $k \neq i,j$

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- Similarly, if $a^{(k-1)}$ is standardized, $\boldsymbol{g}_k^{(t)} = \frac{\partial C}{\partial w^{(k)}}(\Theta^{(t)})$ is more likely to decrease C

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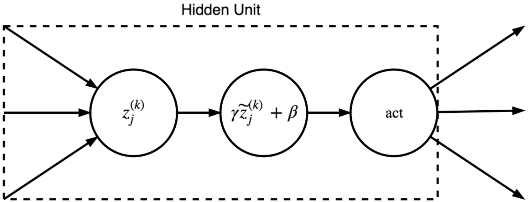
- A hidden unit now looks like:



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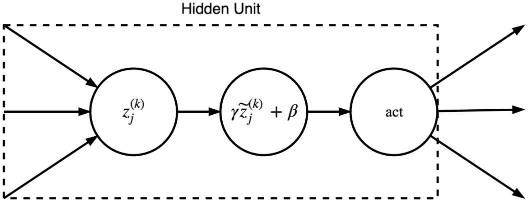
- Observe that there is no need to insist a $\tilde{z}^{(k)}$ to have zero mean and unit variance
  - We only care about whether it is "fixed" when calculating the gradients for other layers

Expressiveness II



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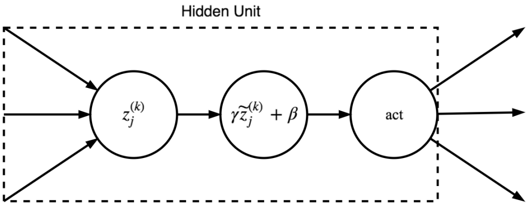

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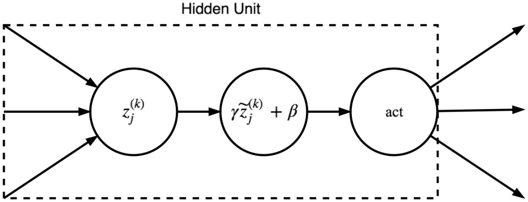

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4. Encode domain-specific knowledge: manifolds, CNNs, RNNs

Regularization in Deep Learning I

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- In these domains, the best fitting model (with lowest generalization error) is usually a larger model regularized appropriately

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- A deep NN is likely to separate a dataset and has the similar issue

Outline

1. Optimization
   - Momentum & Nesterov Momentum
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   - Continuation Methods & Curriculum Learning
   - Cyclic Learning Rates
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- Limiting column norms $\Omega(\boldsymbol{W}^{(k)}_{:,j})$, $\forall j,k$, is preferred [5]
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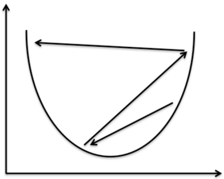
- Prevents ***dead units*** that do not contribute much to the behavior of NN due to too small weights
  - Explicit constraints does not push weights to the origin

Explicit Weight Decay II



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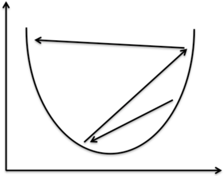

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- Hinton et al. [5] recommend using:

$$\text{explicit constraints} + \text{reprojection} + \text{large learning rate}$$

to allow rapid exploration of parameter space while maintaining numeric stability

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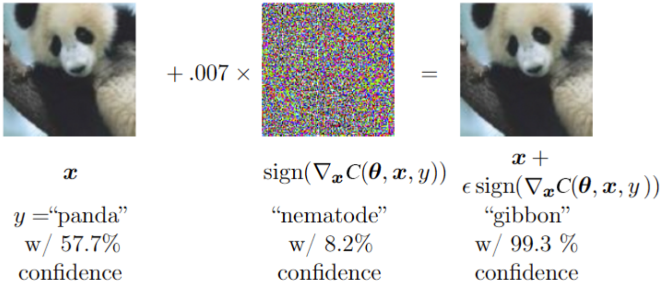
- E.g., in OCR tasks, avoid:
  - Horizontal flips for 'b' and 'd'
  - 180° rotations for '6' and '9'

Noise and Adversarial Data

- NNs are ***not*** very robust to the perturbation of input ($\boldsymbol{x}^{(i)}$'s)
  - Noises [12]
  - Adversarial points [3]



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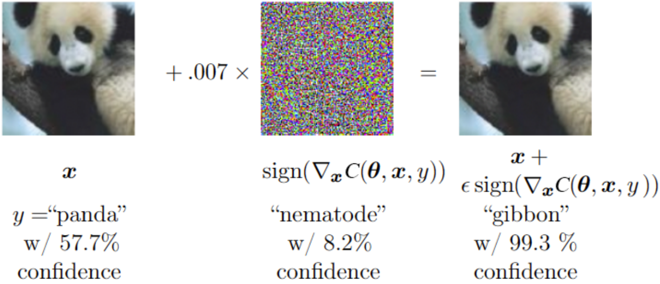

- How to improve the robustness?

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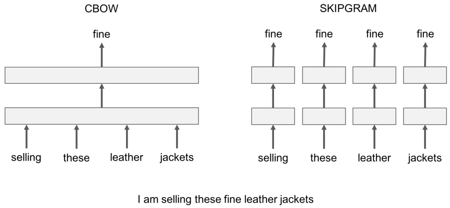
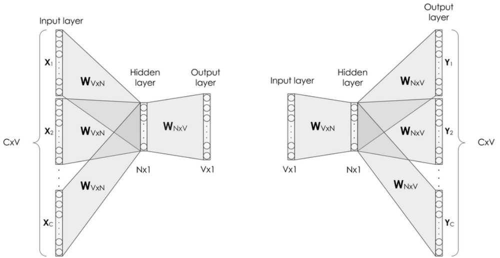
- ***Self-Supervised learning***: learning the structure of $\mathbf{x}$ via $\{\boldsymbol{x}^{(i)}\}_i$ by creating ***virtual labels***

Example: Word2vec Language Model

- ***Contrastive loss*** for a virtual multi-lass classification task:
  - Positive examples: ("I", "am"), ("am", "selling"), ("selling", "fine"), ...
  - Negative examples: ("I", "dog"), ("I", "cat"), ...
- Models & weight tying:





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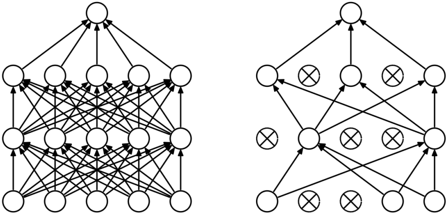

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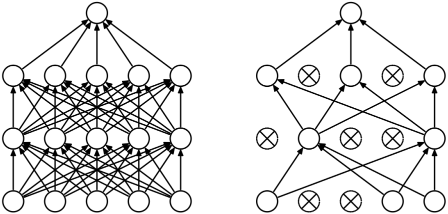

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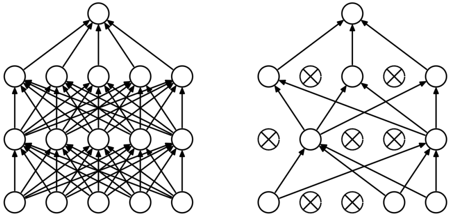

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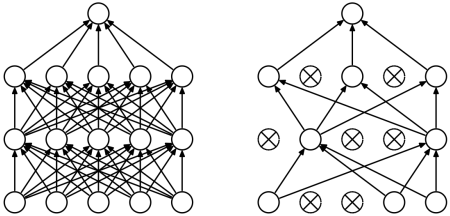

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  - No need to retrain unmasked units
  - Exponential number of voters

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- For example, in face image recognition:
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- Dropping the unit encourages the model to learn mouth (or nose again) in another unit

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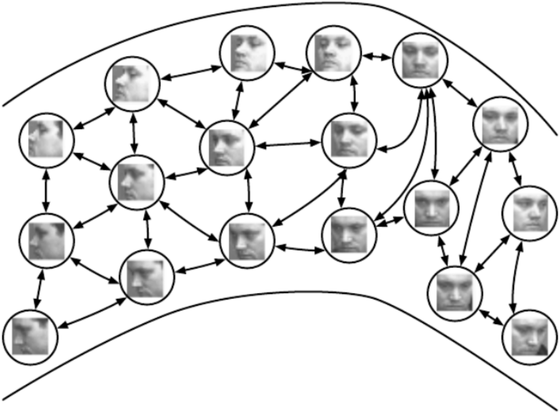
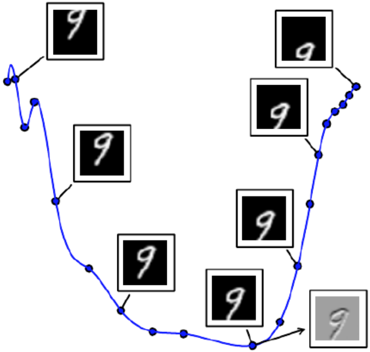
- A manifold is a topological space that are ***linear locally***



Manifolds II

- For each point $\boldsymbol{x}$ on a manifold, we have its ***tangent space*** spanned by ***tangent vectors***
  - Local directions specify how one can change $\boldsymbol{x}$ infinitesimally while staying on the manifold



Tangent Prop

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- Suppose we have the tangent vectors $\{\boldsymbol{v}^{(i,j)}\}_j$ for each example $\boldsymbol{x}^{(i)}$
- Tangent Prop [9] trains an NN classifier f with cost penalty:

$$\Omega[f] = \sum_{i,j} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^{(i)})^\top \boldsymbol{v}^{(i,j)}$$

  - To make f ***local constant along tangent directions***

Tangent Prop

- How to incorporate the manifold prior into a model?
- Suppose we have the tangent vectors $\{\boldsymbol{v}^{(i,j)}\}_j$ for each example $\boldsymbol{x}^{(i)}$
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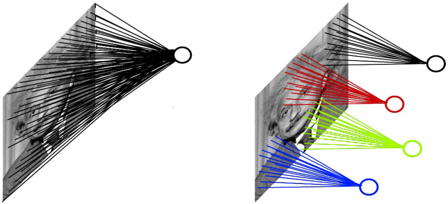
- Manually specified based on domain knowledge
  - Images: scaling, translating, rotating, flipping etc.
- Or learned automatically (to be discussed later)

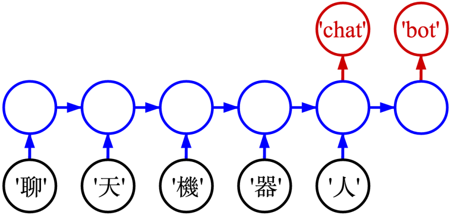
Outline

Domain-Specific Models

- ***Convolutional Neural Networks*** (CNNs) for image processing:



- ***Recurrent Neural Networks*** (RNNs) for sequential data (e.g., natural language) processing:



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