Neural Networks: Optimization & Regularization

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Machine Learning

Outline

1. **Optimization**
   - Momentum & Nesterov Momentum
   - AdaGrad & RMSProp
   - Batch Normalization
   - Continuation Methods & Curriculum Learning
2. **Regularization**
   - Weight Decay
   - Data Augmentation
   - Dropout
   - Manifold Regularization
   - Domain-Specific Model Design

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- NN a complex function:

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

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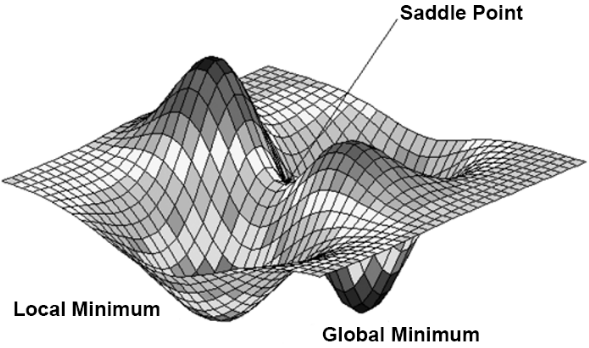
- What are the challenges of solving this problem with SGD?

Non-Convexity

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



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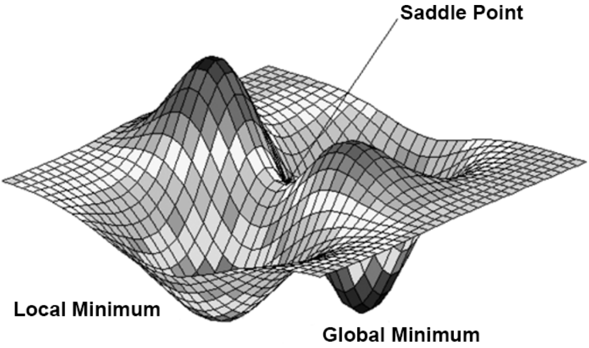

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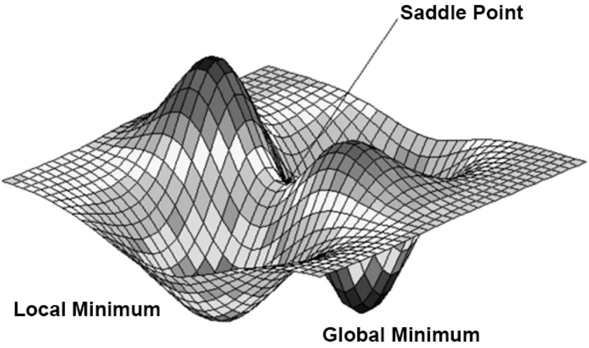

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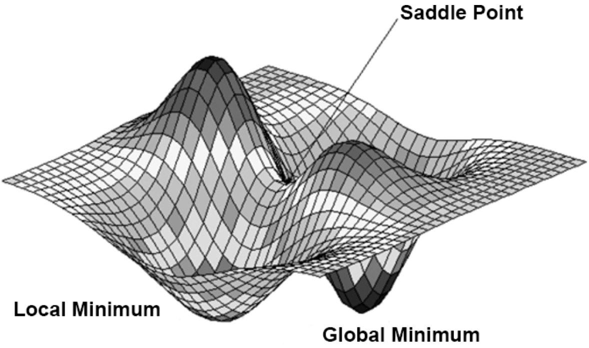

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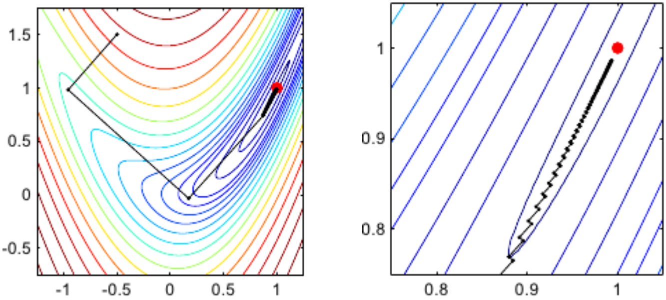
- However, studies [2, 4] show SGD seldom encounters critical points when training a large NN

Ill-Conditioning

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



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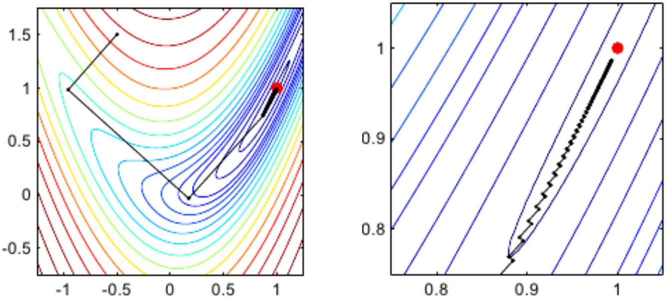

- SGD has slow progress at valleys or plateaus

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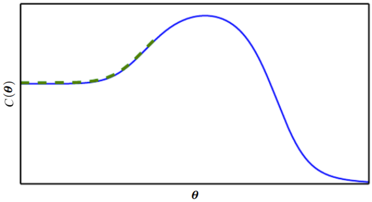
- SGD may proceed along a direction forever
- ***Initialization*** is important



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   - Prevents overfitting

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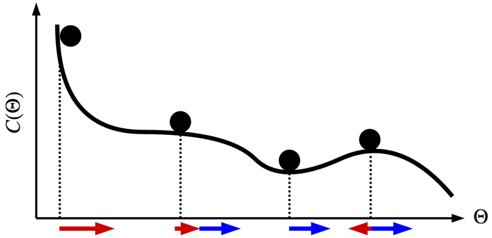
Momentum

- Update rule in SGD:

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

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



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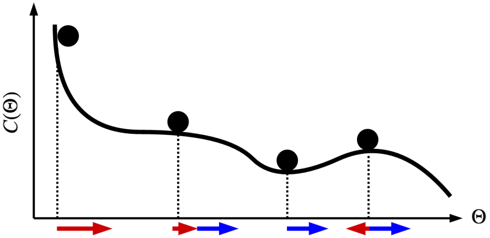

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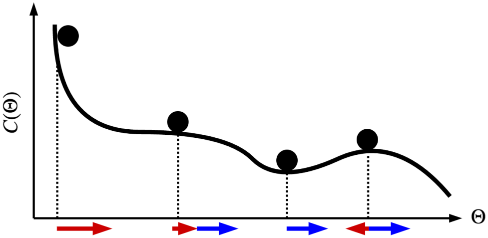
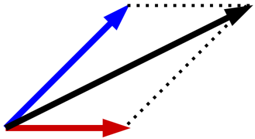


- Momentum: make the same movement $\boldsymbol{v}^{(t)}$ in the last iteration, corrected by negative gradient:

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

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



- $\boldsymbol{v}^{(t)}$ 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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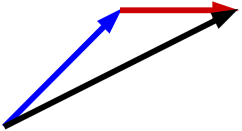

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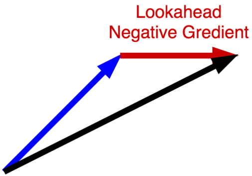

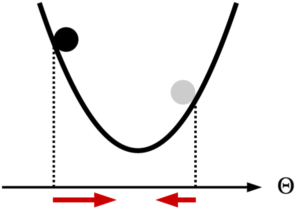

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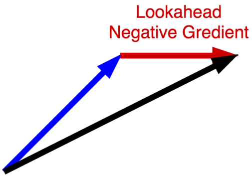
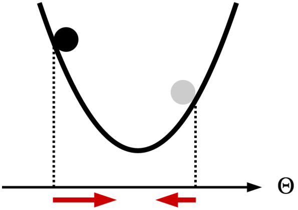
- Faster convergence to a minimum
- Not helpful for NNs that lack of minima





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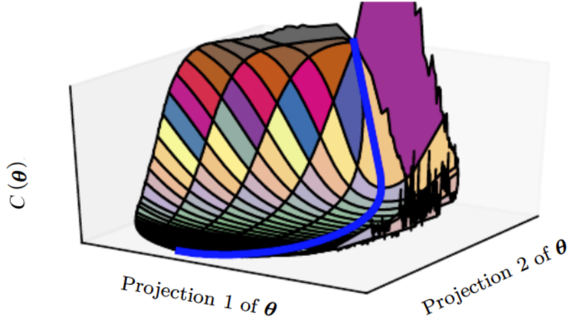
Where Does SGD Spend Its Training Time?



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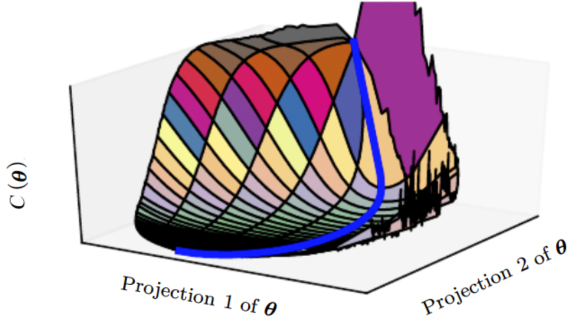
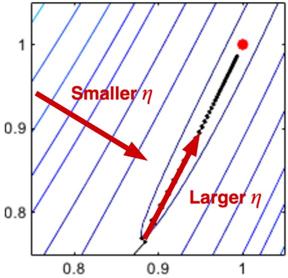


1. Detouring a saddle point of high cost
   - Better initialization
2. Traversing the relatively flat valley
   - Adaptive learning rate

SGD with Adaptive Learning Rates



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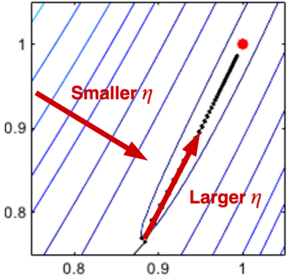

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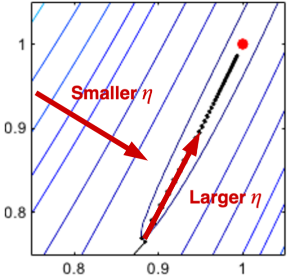

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- How?

AdaGrad

- Update rule:

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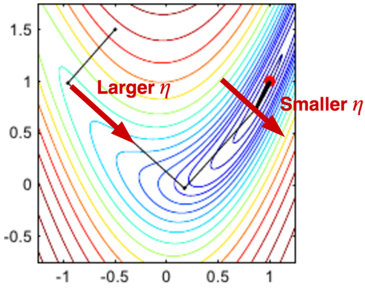
2. ***Larger learning rate along more gently sloped directions***

Limitations



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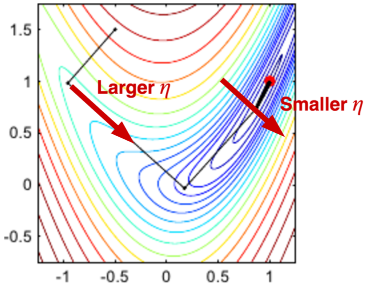

- The optimal learning rate along a direction may ***change over time***
- In AdaGrad, $\boldsymbol{r}^{(t+1)}$ accumulates squared gradients ***from the beginning of training***
  - Results in premature adaptivity

RMSProp

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

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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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- Can we modify the model to ease the optimization task?
- What are the difficulties in training a deep NN?

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- The output $\hat{y}$ is a linear function of x, but ***not*** of weights
- 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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- Can we change the model to make this assumption not-so-wrong?

Batch Normalization I

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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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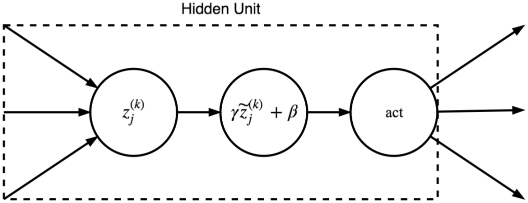
- A hidden unit now looks like:



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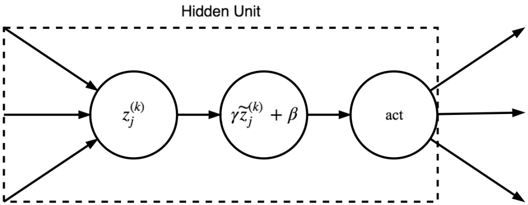
- Observe that there is no need to insist a $\tilde{z}^{(k)}$ to have zero mean and unit variance
  - We only care about whether it is "fixed" when calculating the gradients for other layers

Expressiveness II



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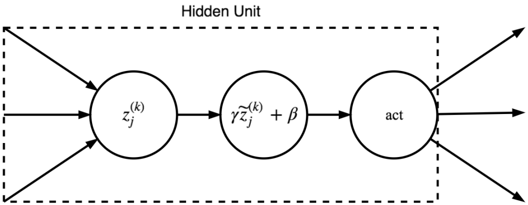

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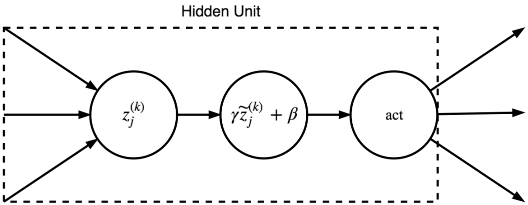

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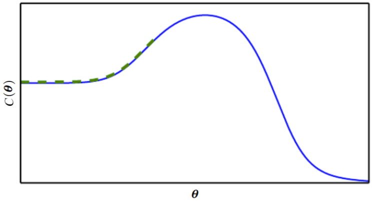
  - The weights $\boldsymbol{W}^{(k)}$, γ, and β are now easier to learn with SGD

Outline

1. **Optimization**
   - Momentum & Nesterov Momentum
   - AdaGrad & RMSProp
   - Batch Normalization
   - Continuation Methods & Curriculum Learning
2. **Regularization**
   - Weight Decay
   - Data Augmentation
   - Dropout
   - Manifold Regularization
   - Domain-Specific Model Design

Parameter Initialization

- ***Initialization*** is important



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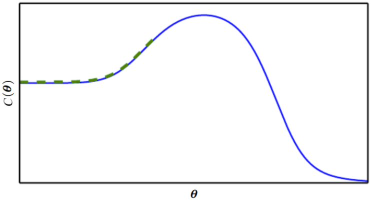

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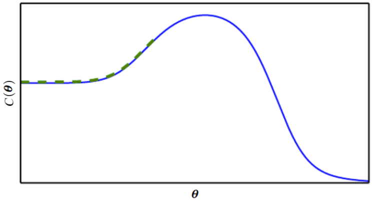

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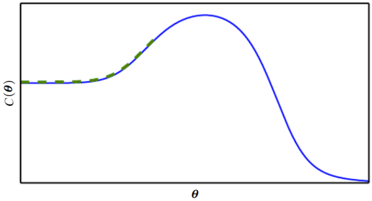


- How to better initialize $\Theta^{(0)}$?

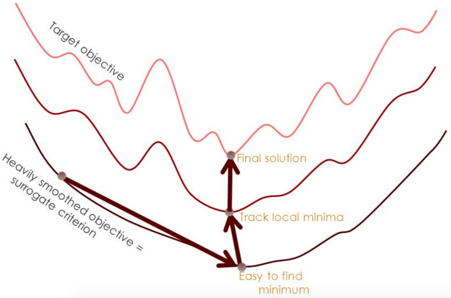
1. Train an NN multiple times with random initial points, and then pick the best
2. Design a series of cost functions such that a solution to one is a good initial point of the next
   - Solve the "easy" problem first, and then a "harder" one, and so on

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



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

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- For "easy" problems, regularization may be necessary to make the problems well defined
- For example, when applying a logistic regression to a linearly separable dataset:

$$\begin{aligned}&\arg\max_{\boldsymbol{w}} \log \textstyle\prod_i \mathrm{P}(y^{(i)} \,|\, \boldsymbol{x}^{(i)}; \boldsymbol{w})\\ = &\arg\max_{\boldsymbol{w}} \log \textstyle\prod_i \sigma(\boldsymbol{w}^\top (i))^{y^{(i)}} [1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}^{(i)})]^{(1-y^{(i)})}\end{aligned}$$

  - If a weight vector $\boldsymbol{w}$ is able to achieve perfect classification, so is $2\boldsymbol{w}$
  - Furthermore, $2\boldsymbol{w}$ gives higher likelihood
  - Without regularization, SGD will continually increase $\boldsymbol{w}$'s magnitude
- A deep NN is likely to separable a dataset and has the similar issue

Outline

Weight Decay

- To add norm penalties:

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- Limiting column norms $\Omega(\boldsymbol{W}^{(k)}_{:,j})$, $\forall j,k$, is preferred [5]
  - Prevents any one hidden unit from having very large weights and $z^{(k)}_j$

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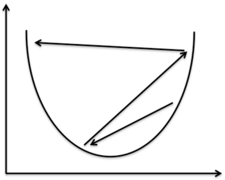
- Prevents ***dead units*** that do not contribute much to the behavior of NN due to too small weights
  - Explicit constraints does not push weights to the origin

Explicit Weight Decay II



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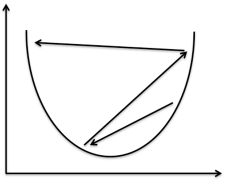

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- Hinton et al. [5] recommend using:

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

to allow rapid exploration of parameter space while maintaining numeric stability

Outline

1. Optimization
   - Momentum & Nesterov Momentum
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2. Regularization
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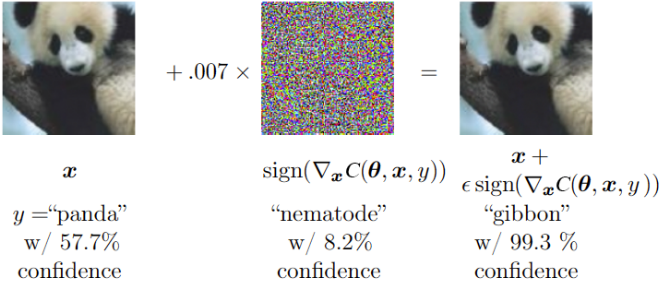
- E.g., in OCR tasks, avoid:
  - Horizontal flips for 'b' and 'd'
  - 180° rotations for '6' and '9'

Noise and Adversarial Data

- NNs are ***not*** very robust to the perturbation of input ($\boldsymbol{x}^{(i)}$'s)
  - Noises [11]
  - Adversarial points [3]



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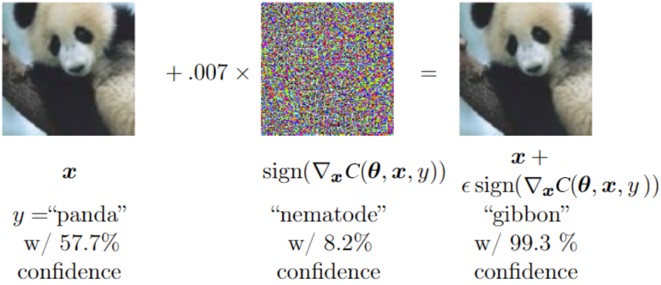

- How to improve the robustness?

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  - Already done in probabilistic models

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- Very time consuming to ensemble a large number of NNs

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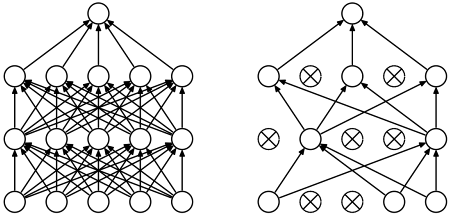

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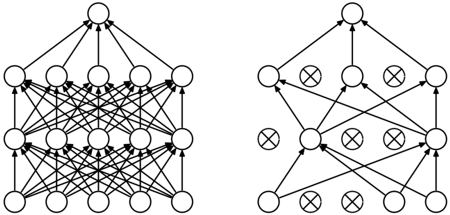

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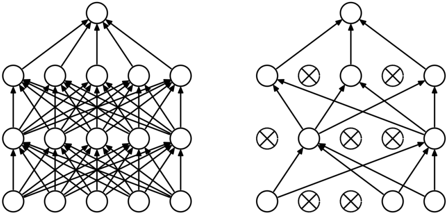

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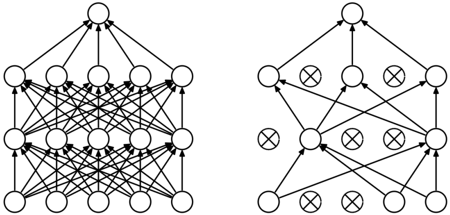

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  - No need to retrain unmasked units
  - Exponential number of voters

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- The better one is problem dependent

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- Dropping the unit encourages the model to learn mouth (or nose again) in another unit

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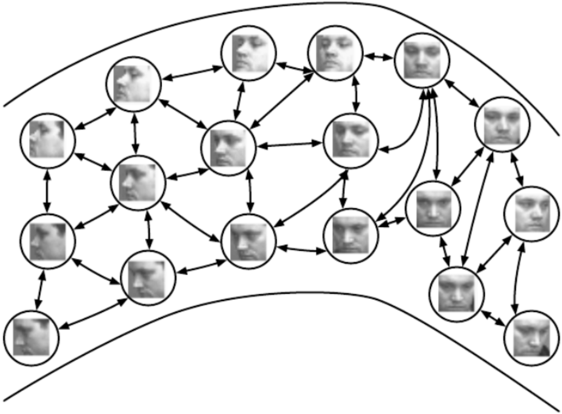
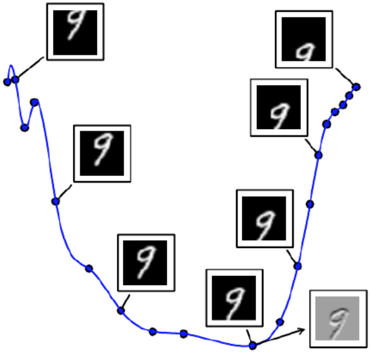
- In many applications, data of the same class concentrate around one or more low-dimensional ***manifolds***
- A manifold is a topological space that are ***linear locally***



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



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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:

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  - Images: scaling, translating, rotating, flipping etc.
- Or learned automatically (to be discussed later)

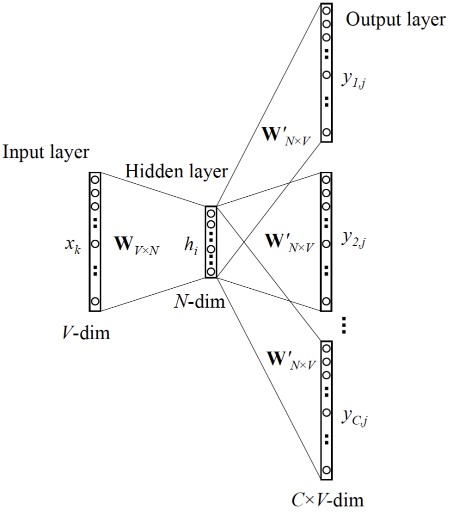
Outline

Domain-Specific Prior Knowledge

- If done right, incorporating the domain-specific prior knowledge into a model is a highly effective way the improve generalizability
  - Better f that "makes sense"
  - May also simplify optimization problem

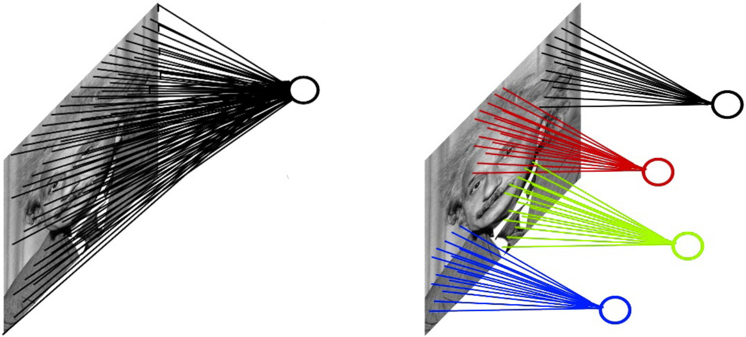
Word2vec

- ***Weight-tying*** leads to simpler model



Convolution Neural Networks

- ***Locally connected*** neurons for pattern detection at different locations



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