# Neural Networks: Optimization & Regularization

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Machine Learning

# Outline

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

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# Challenges

- NN a complex function:

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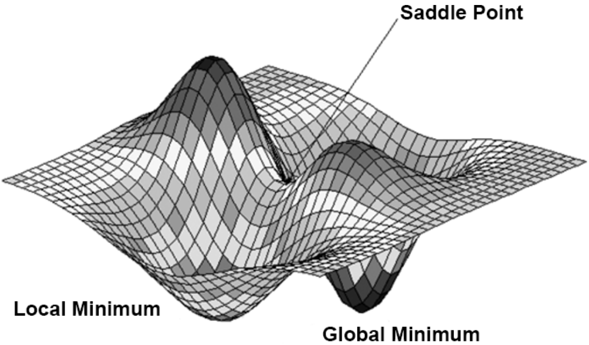
- What are the challenges of solving this problem with SGD?

# Non-Convexity

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



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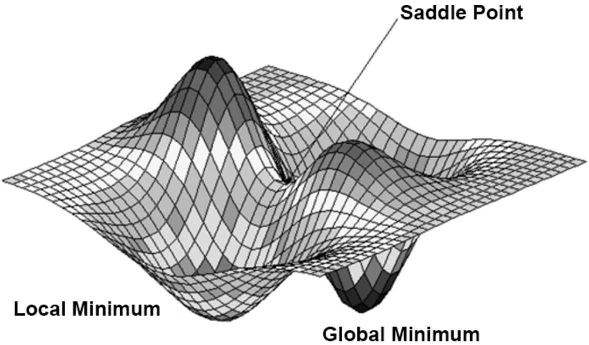


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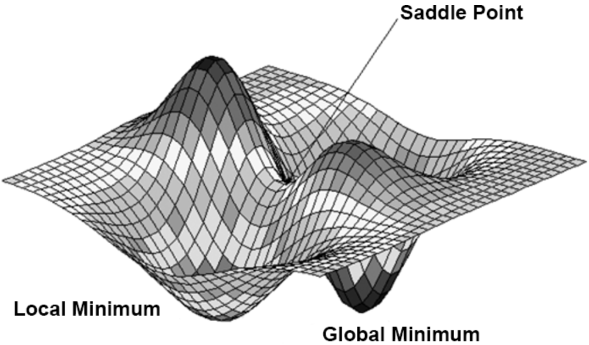


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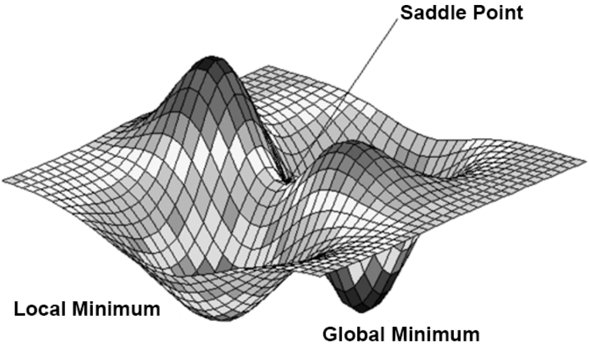


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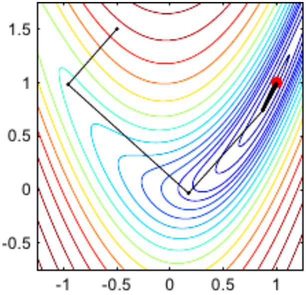
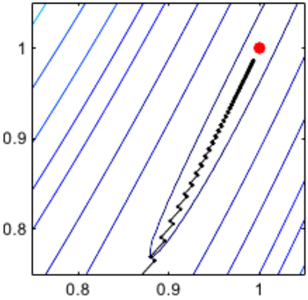
- However, studies [2, 4] show SGD seldom encounters critical points when training a large NN

# Ill-Conditioning

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



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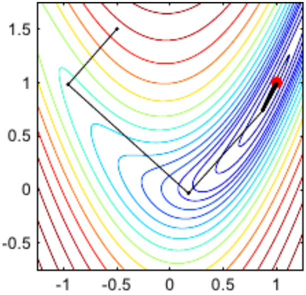


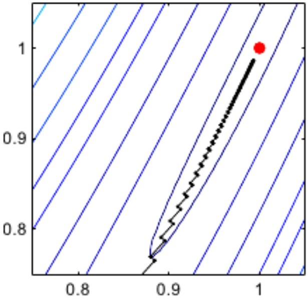


- SGD has slow progress at valleys or plateaus

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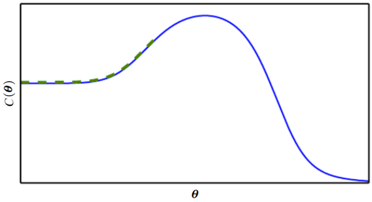
- SGD may proceed along a direction forever
- ***Initialization*** is important



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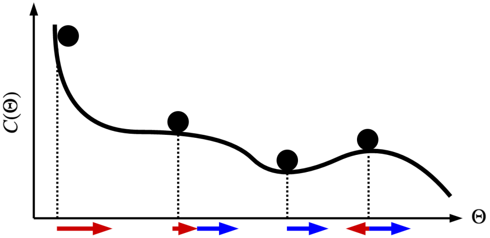
# Momentum

- 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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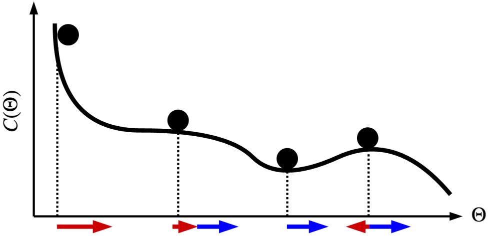

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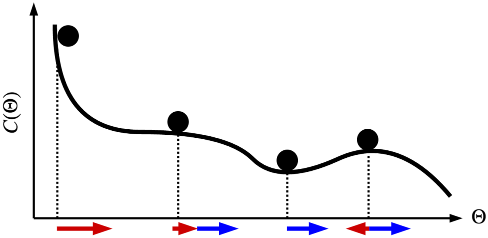


- Momentum: make the same movement $\boldsymbol{v}^{(t)}$ in the last iteration, corrected by negative gradient:

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

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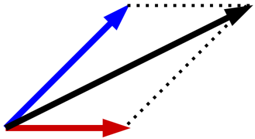


- $\boldsymbol{v}^{(t)}$ is a moving average of $-\boldsymbol{g}^{(t)}$

# Nesterov Momentum

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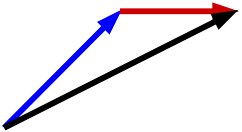

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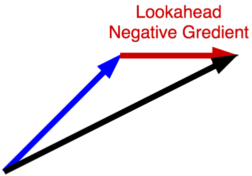


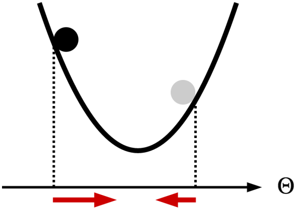

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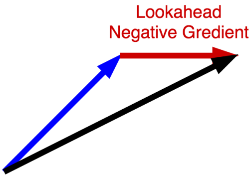
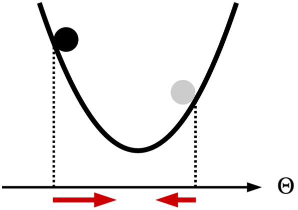
- Not helpful for NNs that lack of minima



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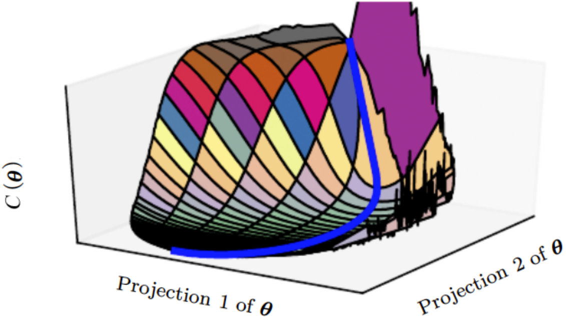
# Where Does SGD Spend Its Training Time?



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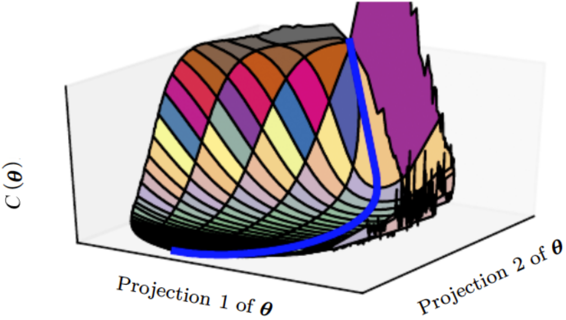
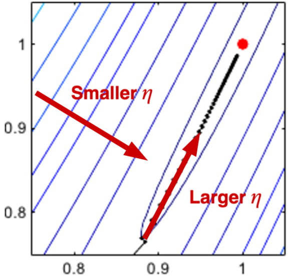



1. Detouring a saddle point of high cost
   - Better initialization
2. Traversing the relatively flat valley
   - Adaptive learning rate

# SGD with Adaptive Learning Rates

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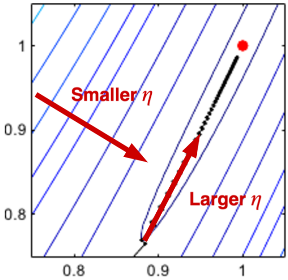


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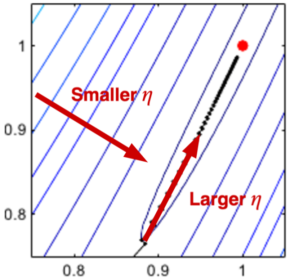


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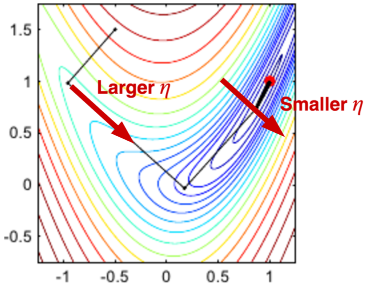
2. ***Larger learning rate along more gently sloped directions***

# Limitations

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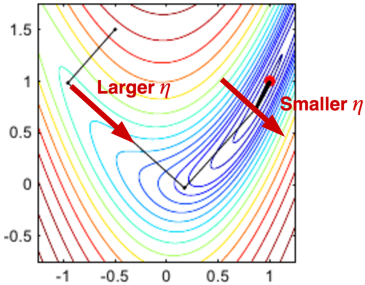


- The optimal learning rate along a direction may ***change over time***
- In AdaGrad, $\boldsymbol{r}^{(t+1)}$ accumulates squared gradients ***from the beginning of training***
  - Results in premature adaptivity

# 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:

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

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

$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} + \frac{\eta}{\sqrt{\boldsymbol{r}^{(t+1)}}} \odot \boldsymbol{v}^{(t+1)}$$

  - 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

$$\hat{y} = f(x) = xw^{(1)}w^{(2)}\cdots w^{(L)}$$

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- Can be readily extended to NNs having multiple neurons at each layer

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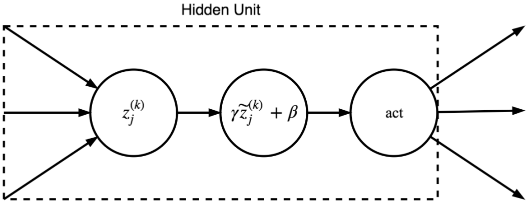
- A hidden unit now looks like:



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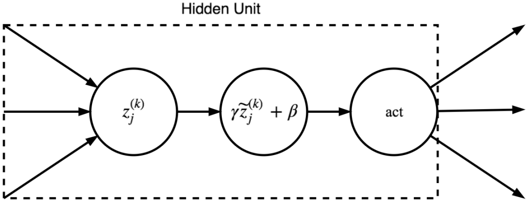
- But at the cost of expressiveness
  - Normalizing $a^{(k)}$ or $z^{(k)}$ limits the output range of a unit
- Observe that there is no need to insist a $\tilde{z}^{(k)}$ to have zero mean and unit variance
  - We only care about whether it is "fixed" when calculating the gradients for other layers

# Expressiveness II

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to learn their best values

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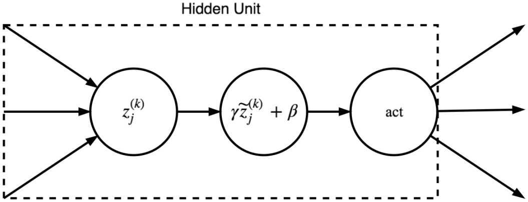


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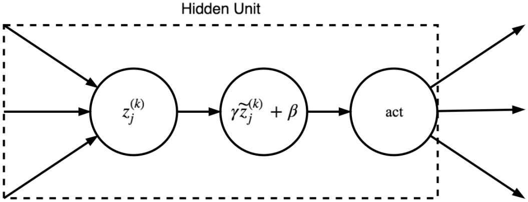


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  - The weights $\boldsymbol{W}^{(k)}$, $\gamma$, and $\beta$ are now easier to learn with SGD

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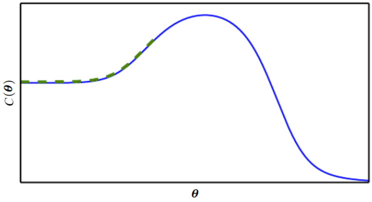
# Parameter Initialization

- *Initialization* is important



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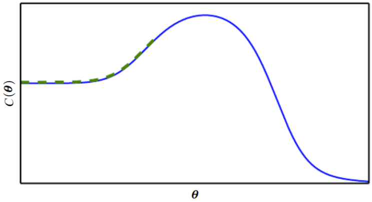


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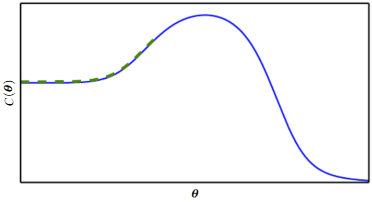


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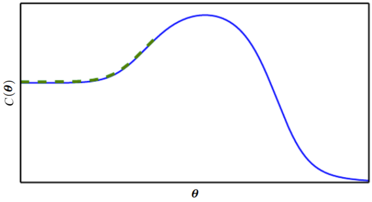



- How to better initialize $\Theta^{(0)}$?

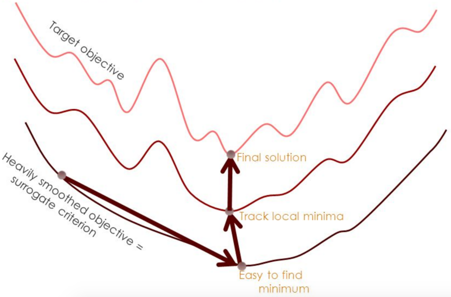
1. Train an NN multiple times with random initial points, and then pick the best
2. Design a series of cost functions such that a solution to one is a good initial point of the next
   - Solve the "easy" problem first, and then a "harder" one, and so on

# 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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- Cost function might not become convex, no matter how much it is smoothen
- 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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# Prior Predictions of NTK-GP

- Prior (unconditioned) mean predictions for training set:

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

- Prior mean predictions for test set:

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

- 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

# Trainability

- Prior (unconditioned) mean predictions for training set:

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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

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

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

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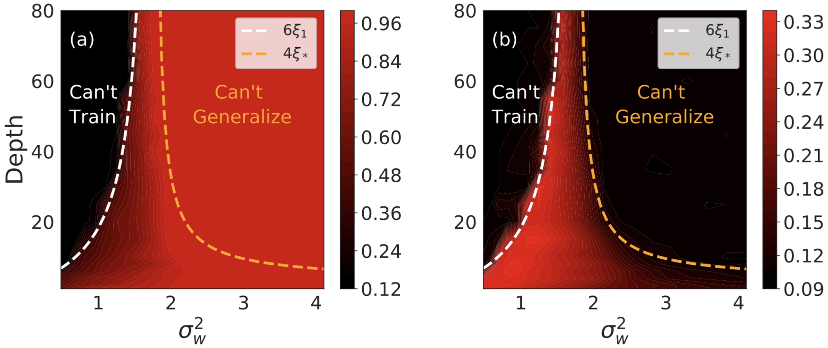
- If $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}$ ***is a data-independent constant matrix***, then the NN will fail to generalize
    - If $\boldsymbol{y}$ has zero mean, this implies that $\boldsymbol{T}_{M,N}\boldsymbol{T}_{N,N}^{-1}\boldsymbol{y} = \boldsymbol{0}$

# Results

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



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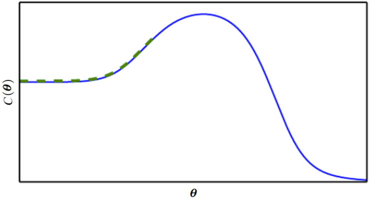
- A deep NN is likely to separable a dataset and has the similar issue

# Outline

# SGD Gradients are Noisy

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



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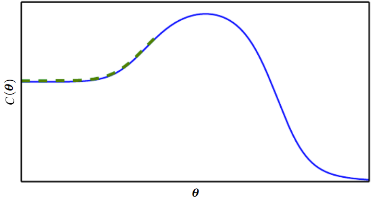
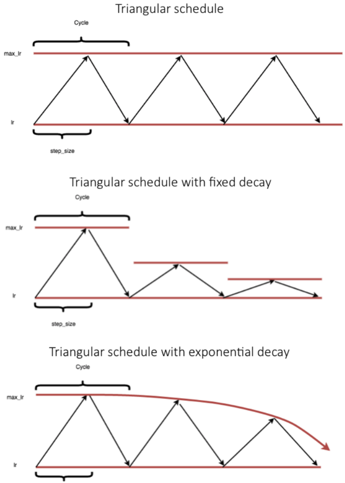



- Use a small learning rate in the very beginning [10]



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- 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 $z_j^{(k)}$

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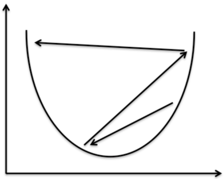
- Prevents ***dead units*** that do not contribute much to the behavior of NN due to too small weights
  - Explicit constraints does not push weights to the origin

# Explicit Weight Decay II



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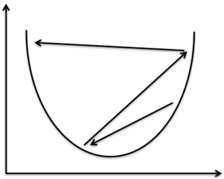

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- Hinton et al. [5] recommend using:

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

  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'
  - $180^\circ$ 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]
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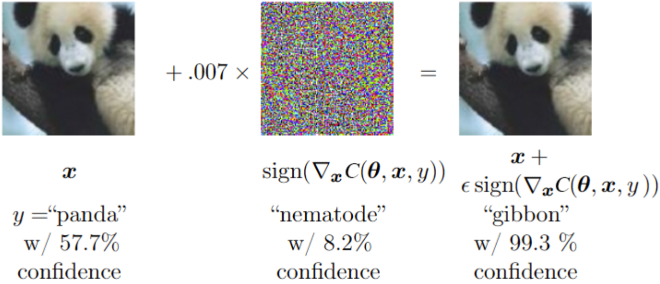

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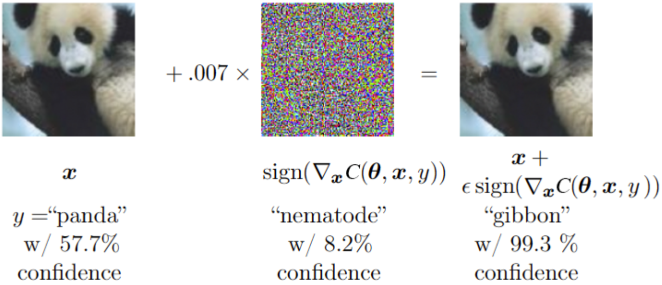


- How to improve the robustness?

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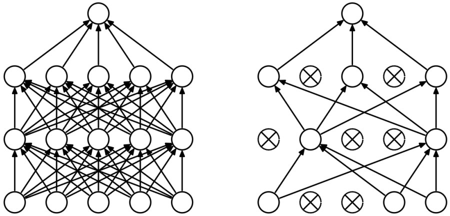

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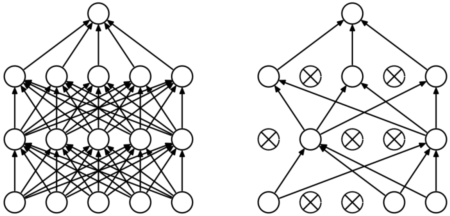

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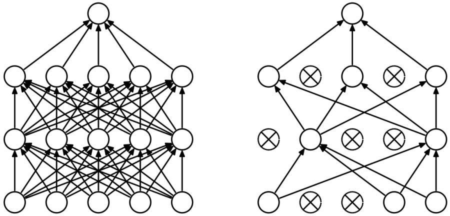

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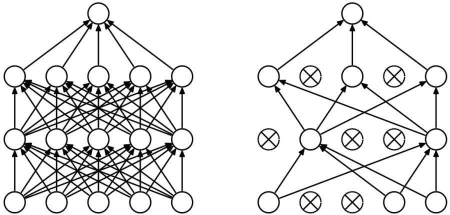

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  - No need to retrain unmasked units
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- Dropping the unit encourages the model to learn mouth (or nose again) in another unit

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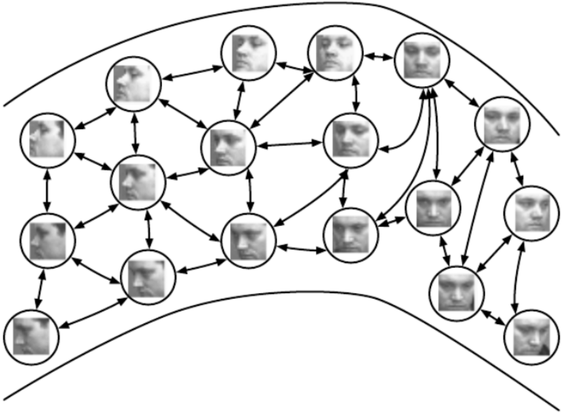
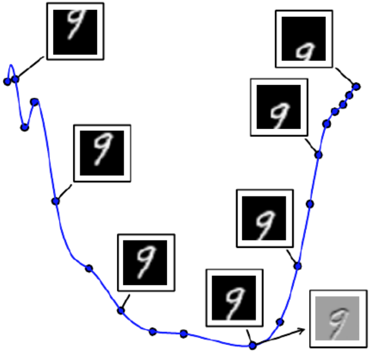
- In many applications, data of the same class concentrate around one or more low-dimensional ***manifolds***
- A manifold is a topological space that are ***linear locally***



# 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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- Manually specified based on domain knowledge
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- Or learned automatically (to be discussed later)

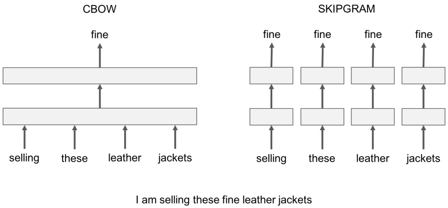
# Outline

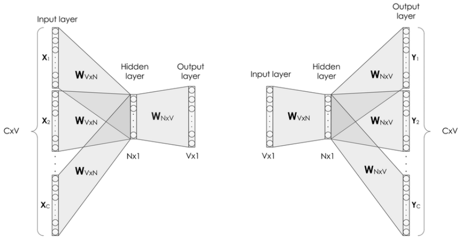
# Domain-Specific Prior Knowledge

- 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

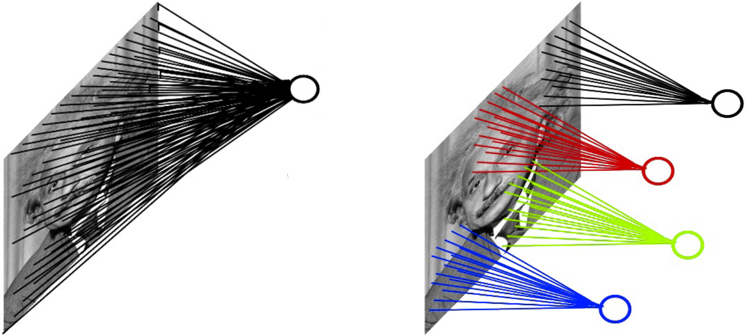
- ***Weight-tying*** leads to simpler model



# Convolution Neural Networks

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



# Reference I

[1] Yoshua Bengio, Jérôme Louradour, Ronan Collobert, and Jason Weston.
Curriculum learning.
In *Proceedings of the 26th annual international conference on machine learning*, pages 41–48. ACM, 2009.

[2] Anna Choromanska, Mikael Henaff, Michael Mathieu, Gérard Ben Arous, and Yann LeCun.
The loss surfaces of multilayer networks.
In *AISTATS*, 2015.

[3] Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy.
Explaining and harnessing adversarial examples.
*arXiv preprint arXiv:1412.6572*, 2014.

[4] Ian J Goodfellow, Oriol Vinyals, and Andrew M Saxe.
Qualitatively characterizing neural network optimization problems.
*arXiv preprint arXiv:1412.6544*, 2014.

# Reference II

[5] Geoffrey E Hinton, Nitish Srivastava, Alex Krizhevsky, Ilya Sutskever, and Ruslan R Salakhutdinov.
Improving neural networks by preventing co-adaptation of feature detectors.
*arXiv preprint arXiv:1207.0580*, 2012.

[6] Sergey Ioffe and Christian Szegedy.
Batch normalization: Accelerating deep network training by reducing internal covariate shift.
*arXiv preprint arXiv:1502.03167*, 2015.

[7] Diederik Kingma and Jimmy Ba.
Adam: A method for stochastic optimization.
*arXiv preprint arXiv:1412.6980*, 2014.

[8] Ben Poole, Jascha Sohl-Dickstein, and Surya Ganguli.
Analyzing noise in autoencoders and deep networks.
*arXiv preprint arXiv:1406.1831*, 2014.

# Reference III


[9] Patrice Simard, Bernard Victorri, Yann LeCun, and John S Denker. Tangent prop-a formalism for specifying selected invariances in an adaptive network. In *NIPS*, volume 91, pages 895–903, 1991.

[10] Leslie N Smith. Cyclical learning rates for training neural networks. In *2017 IEEE Winter Conference on Applications of Computer Vision (WACV)*, pages 464–472. IEEE, 2017.

[11] Christian Szegedy, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, and Andrew Rabinovich. Going deeper with convolutions. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 1–9, 2015.

# Reference IV


[12] Yichuan Tang and Chris Eliasmith.
Deep networks for robust visual recognition.
In *Proceedings of the 27th International Conference on Machine Learning (ICML-10)*, pages 1055–1062, 2010.