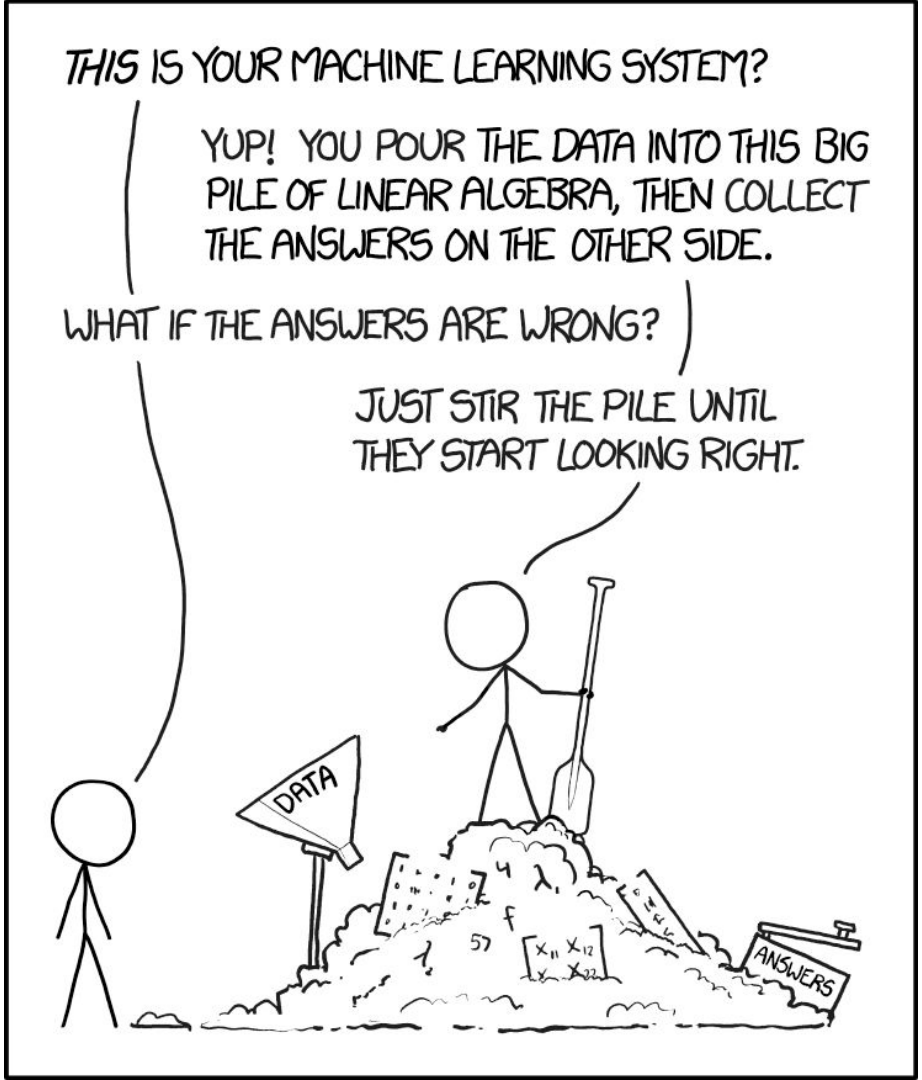
THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

# CIS 522: Lecture 15

Generalization and overfitting
03/05/20

Penn Engineering

# Intro

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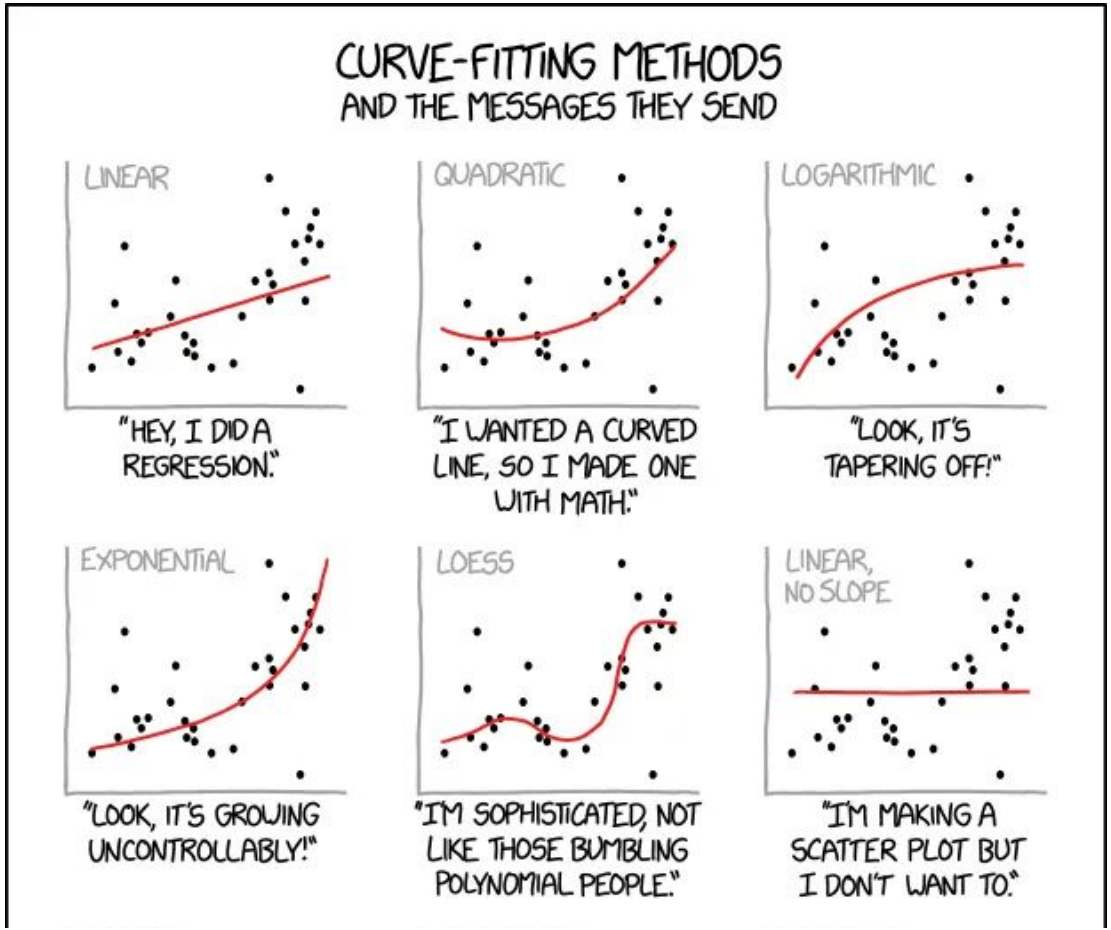
# What is generalization?

- Learn from a training set, evaluate on a test set
- Generalization gap: Difference between loss on training set and test set

# Why is it hard?



# Class 1

# Class 2

# Which class is this?

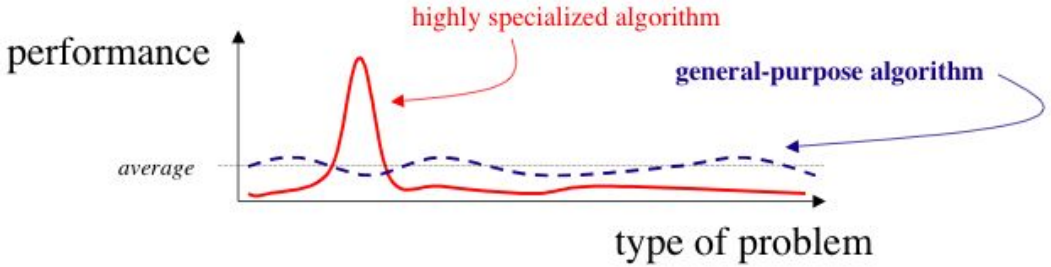
# No free lunch theorem

Theorem: If an algorithm performs better than random search on some class of problems then it **must** perform worse than random search on the remaining problems

In other words:

- A superior black-box optimization strategy is impossible
- If our feature space is unstructured, we can do no better than random
- “A jack of all trades is a master of none”

# No Free Lunch theorem (example)



# Overfitting

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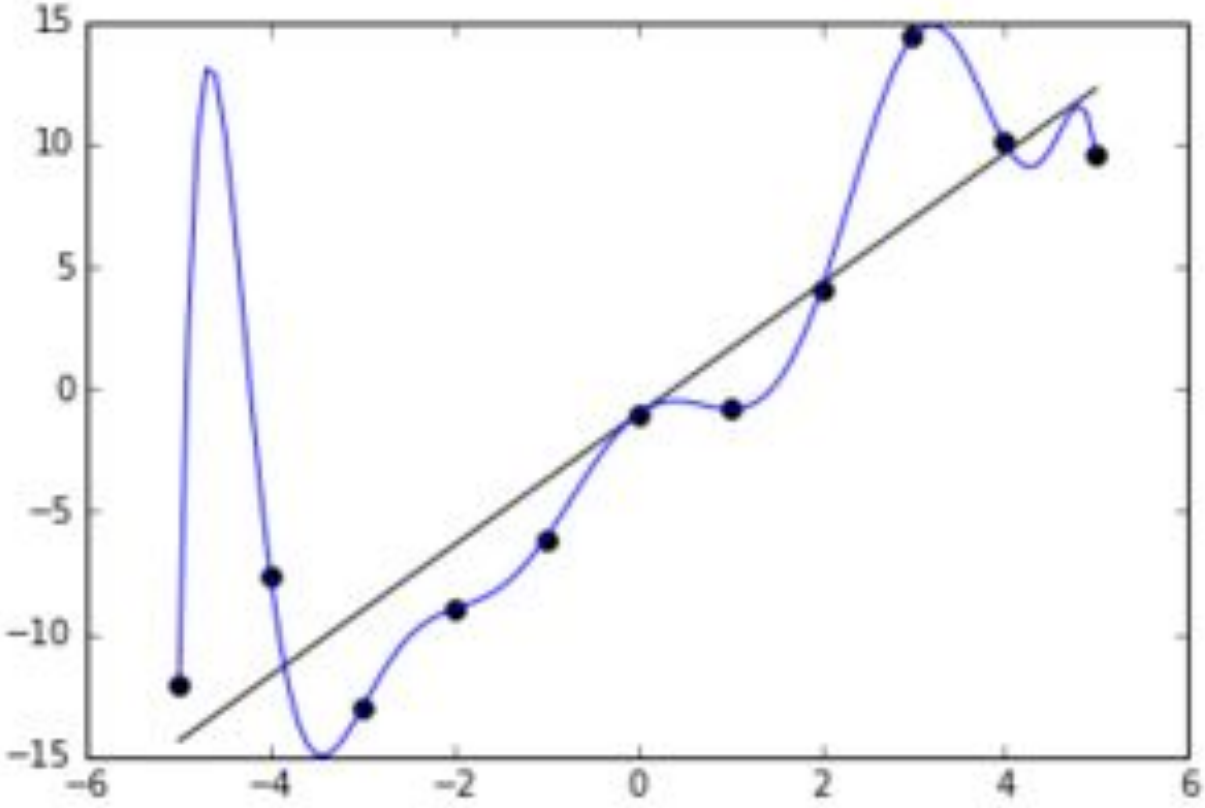
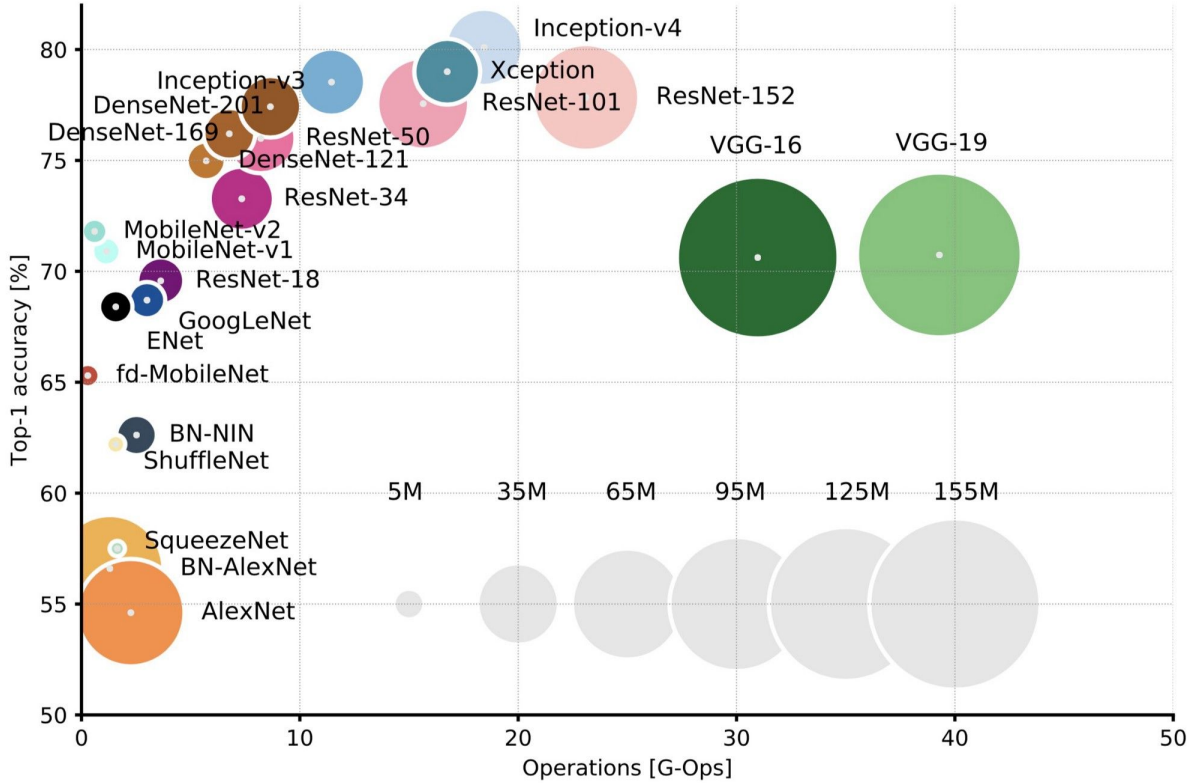
# Overfitting



# Generally if # parameters >> # data

- More parameters means can fit more exactly
- E.g. linear fit vs. higher degree polynomial

# Why don’t neural networks overfit?

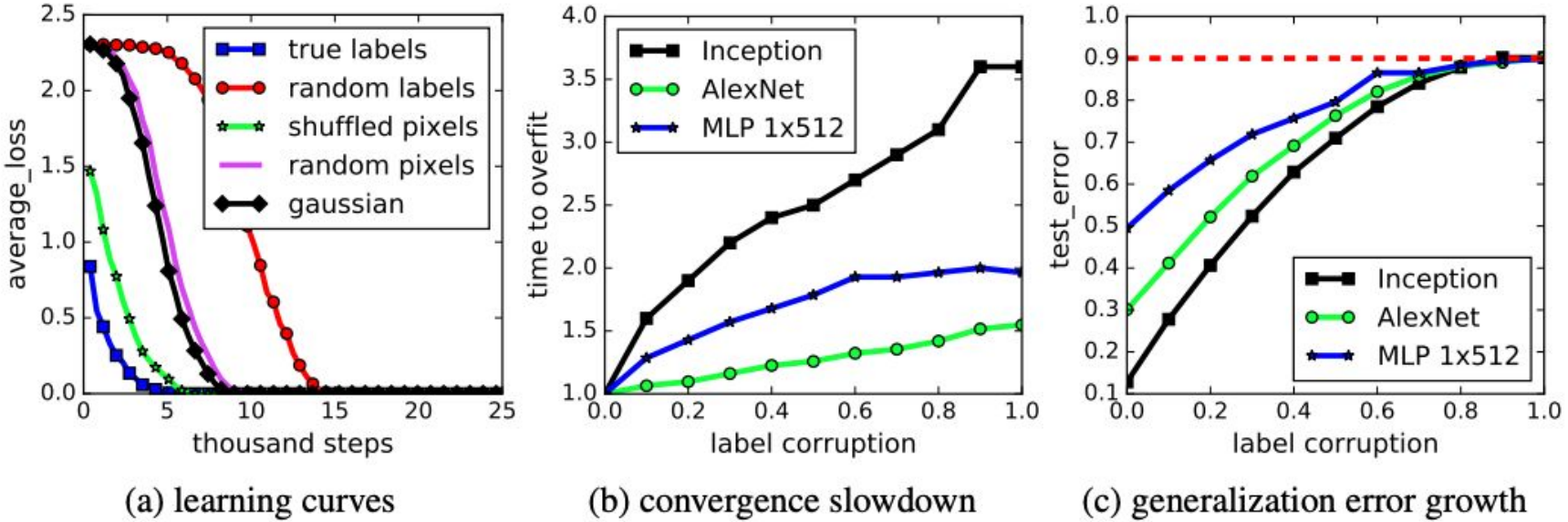


# First answer: they do sometimes

- Train for too long
- Learning rate too small or batch size too large (will explain later)
- Training data doesn't have easily learnable patterns

# Memorization

- Neural networks can learn random labels or random input data
- By definition, no generalization possible



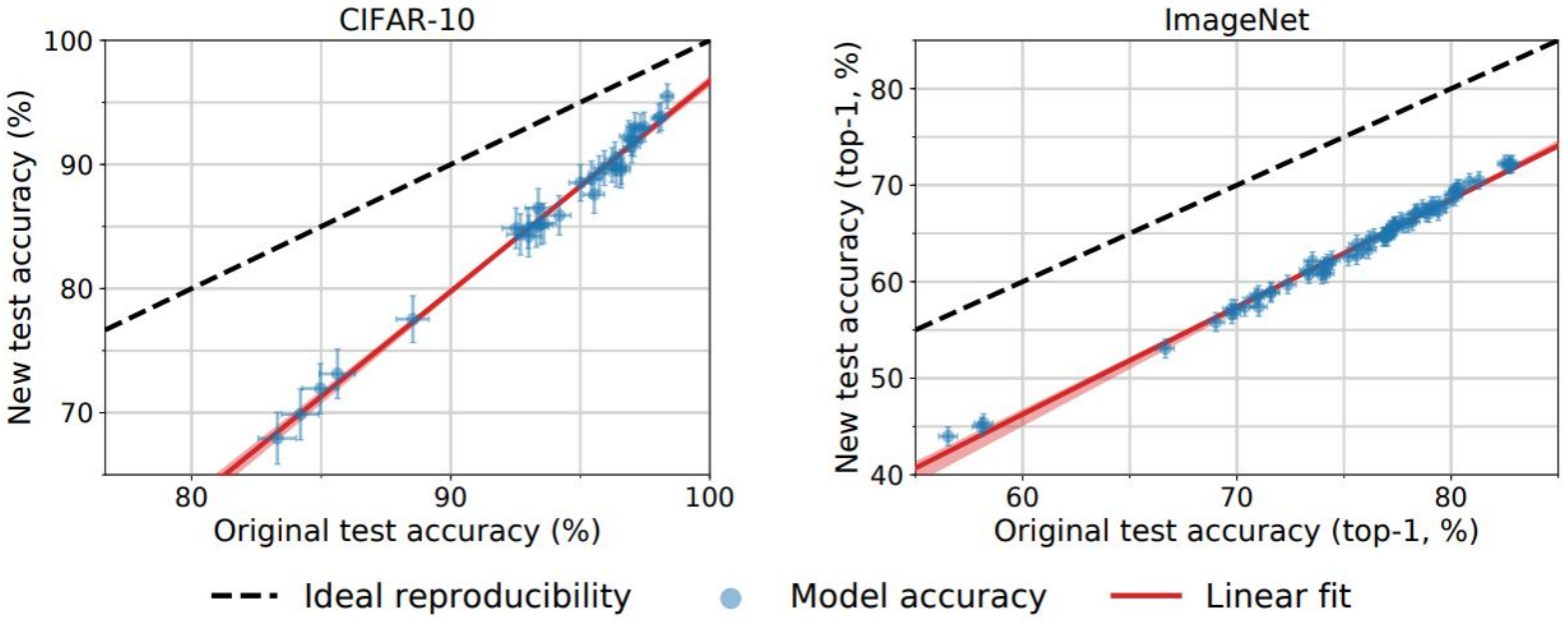

(a) learning curves (b) convergence slowdown (c) generalization error growth

Figure 1: Fitting random labels and random pixels on CIFAR10. (a) shows the training loss of various experiment settings decaying with the training steps. (b) shows the relative convergence time with different label corruption ratio. (c) shows the test error (also the generalization error since training error is 0) under different label corruptions.

"Understanding deep learning requires rethinking generalization", Zhang et al., ICLR 2017

# Meta-overfitting

- Implicitly fitting algorithms to the test datasets




"Do ImageNet Classifiers Generalize to ImageNet?", Recht et al., arXiv 2019.

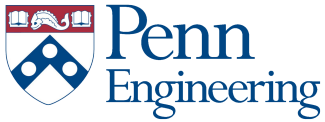
# Generalization before memorization

- See work of Arpit et al. 2017
- Neural nets performance on test set peaks before performance on training set

# Implicitly, we need inductive biases

- E.g. towards lines and other “simple” functions
- Towards spatially coherent objects in images
- Can be hard to specify exactly what inductive biases are right, but neural nets sometimes have them
- Want to understand when nets will generalize and how we can make them generalize better

# Generalization guarantees



# VC dimension

- Suppose F is a set of functions
- Say that F "shatters" a set of n data points if for every possible labeling of the data points, there is some f in F that gets the labeling right
- The VC dimension of F is the maximum n such that F shatters all sets of n data points
- Intuitively: VC dim is size of sets that can be memorized

# VC dimension

- Ideally, we would want deep networks to have small VC dimension - hard to memorize large amounts of data
- But they have huge VC dimension: $\geq$ (# weights)$^2$
- Still generalize pretty well!

# Compressing networks

- Can consider the *effective* size of networks instead
- Many networks can be compressed to smaller networks that perform just as well
- Has been explored also in context of e.g. storing on phones

# How to compress a network

- Train the network
- Prune the low absolute-value weights
- Re-train with those held at zero
- Repeat
- Can often remove ~90% of weights with negligible loss of accuracy

# PAC-Bayes with neural networks

- Data-dependent bounds on generalization
- Can get first non-trivial bounds - e.g. provable ~80% for MNIST
- Still not matching performance, but getting there
- PAC framework: for small $\varepsilon, \delta > 0$, draw function from family F, prove only an $\varepsilon$ chance of more than $\delta$

"Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data", Dziugaite and Roy, UAI 2016

# Preventing overfitting

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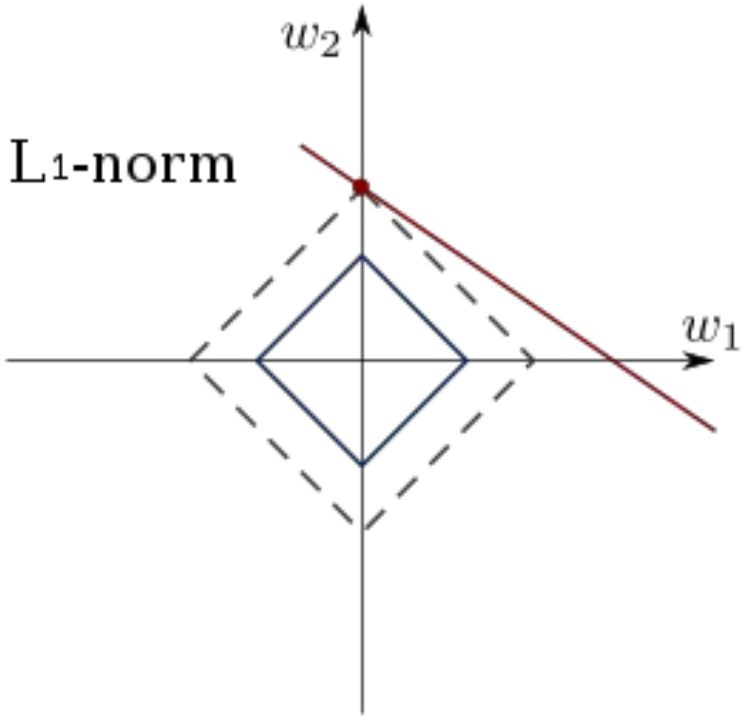
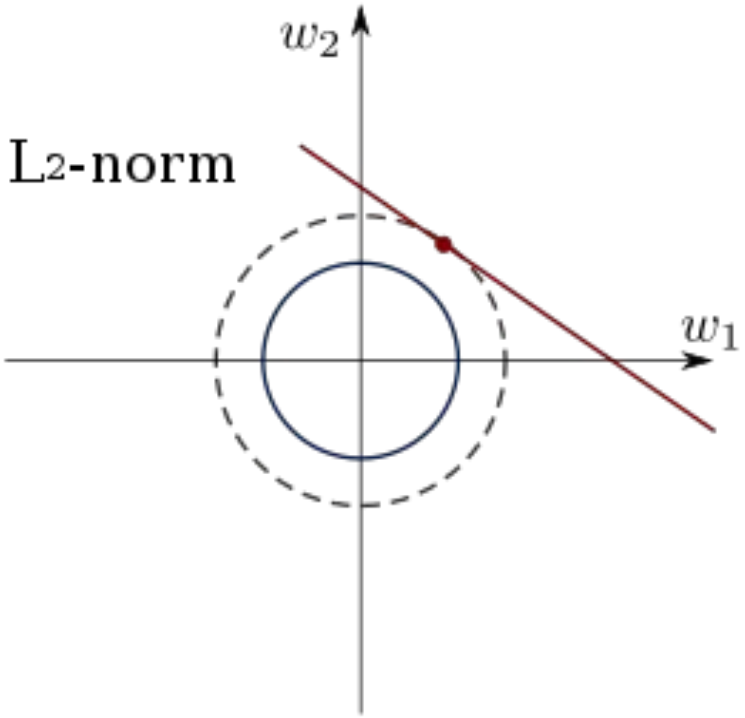
# Regularization

- Train to minimize normal loss + c * L1(weights)
  - Has the effect of driving some weights to 0
  - See lasso regression
- Train to minimize normal loss + c * L2 (weights)
  - Has the effect of making some weights small
  - See ridge regression

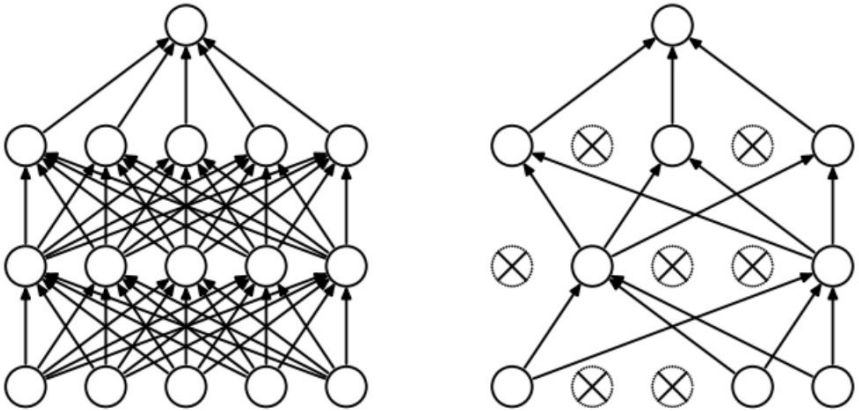
# Regularization



# Dropout

- Recap: Kill some neurons during training time
- Use all neurons during test time



(a) Standard Neural Net

(b) After applying dropout.

# Dropout

- Prevents overfitting by breaking brittle predictions
- Forces "dead branches" to learn
- Enforces distributed nature
- Distributes learning signal
- Adds lots of noise
- In a way approximates ensemble methods

# Implicit regularization - ResNets

- Many paths for information flow through the network
- No one path, or neuron, or layer, is necessary

# Implicit regularization - ResNets

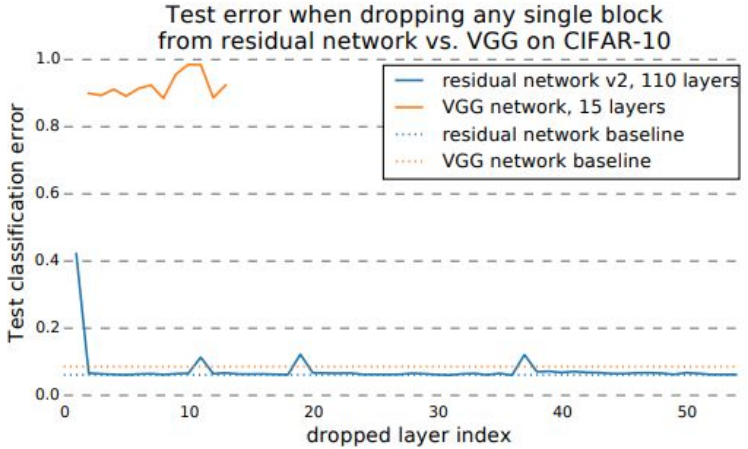



Figure 3: Deleting individual layers from VGG and a residual network on CIFAR-10. VGG performance drops to random chance when any one of its layers is deleted, but deleting individual modules from residual networks has a minimal impact on performance. Removing downsampling modules has a slightly higher impact.

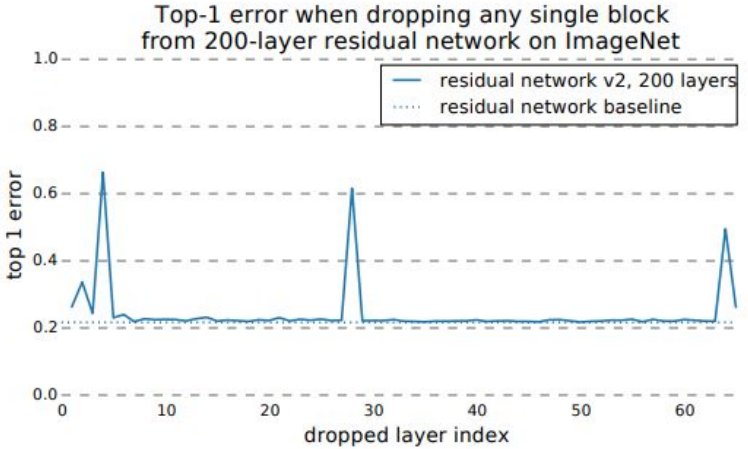



Figure 4: Results when dropping individual blocks from residual networks trained on ImageNet are similar to CIFAR results. However, downsampling layers tend to have more impact on ImageNet.

"Residual Networks Behave Like Ensembles of Relatively Shallow Networks", Veit et al, NeurIPS 2016

# Deep linear networks

- No activation function:

$$W_k \ldots W_2 W_1 x$$

- Seems kinda silly
- Can express only linear functions ($W = W_k \ldots W_2 W_1$)

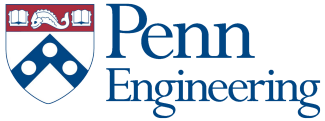
# Implicit regularization - deep linear networks

- But you are running backprop on many weight matrices at once
- Turns out to regularize!

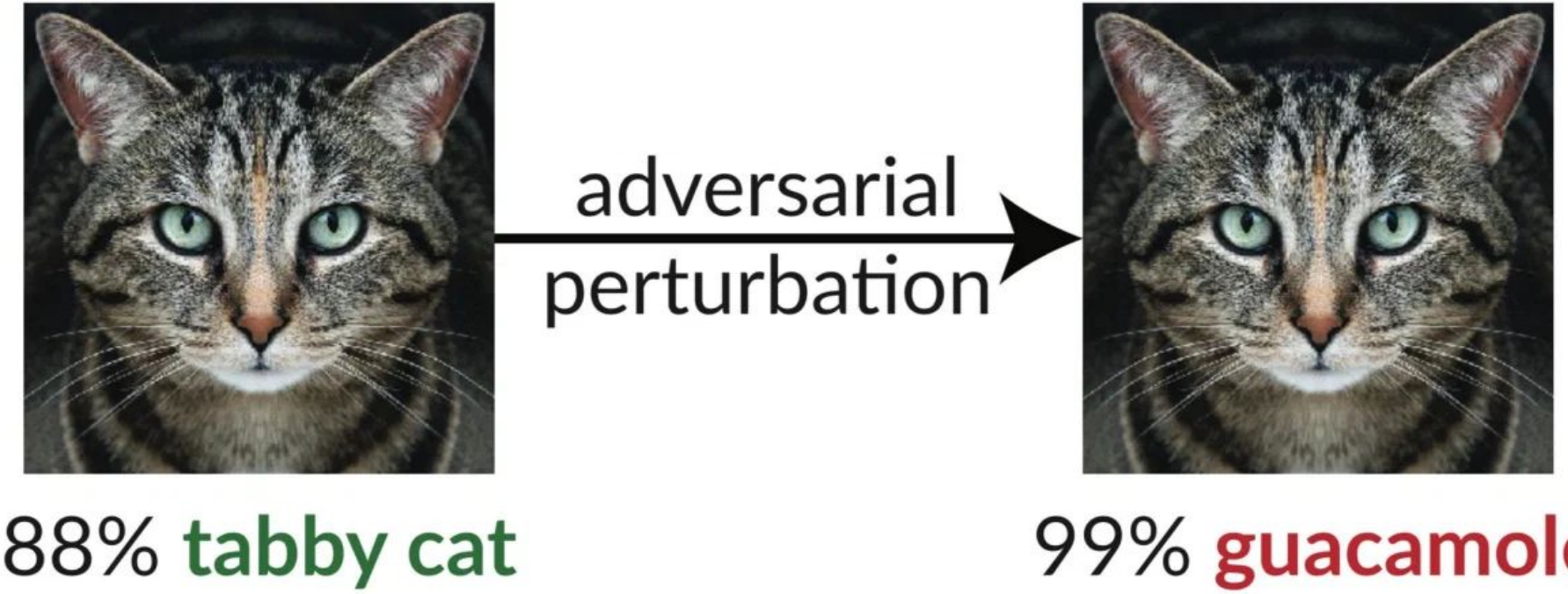
# Example: matrix completion ("Netflix prize")

- Given some entries of a matrix, try to complete the matrix $W$, assuming it has low rank
- Deep linear network: set $W = W_k \ldots W_2 W_1$
- Loss function: difference between predicted entries and given entries + L2 norm of $W_i$
- Proof: in certain cases, converges to $W$ with min nuclear norm (L1 norm of eigenvalues) (Gunasekar et al.)

# Weird properties of large networks



# Adversarial examples



# Adversarial examples

$\boldsymbol{x}$

"panda"
57.7% confidence

$+.007 \times$

$\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

"nematode"
8.2% confidence

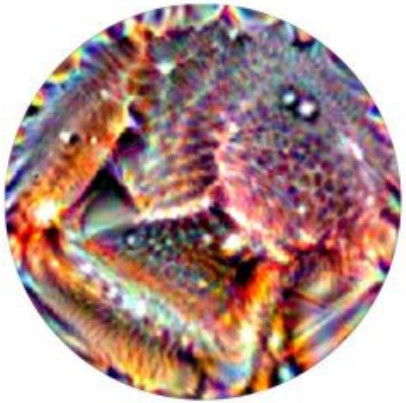
$=$

$\boldsymbol{x} + \epsilon\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$

"gibbon"
99.3 % confidence

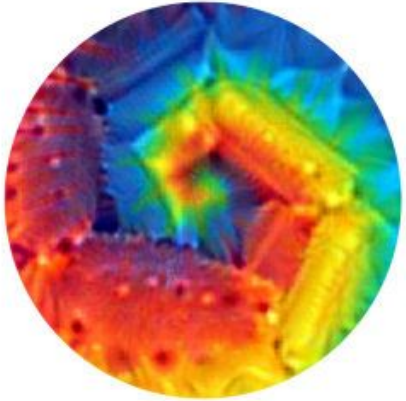

rifle
shield, buck
revolver, si

Banana



Crab

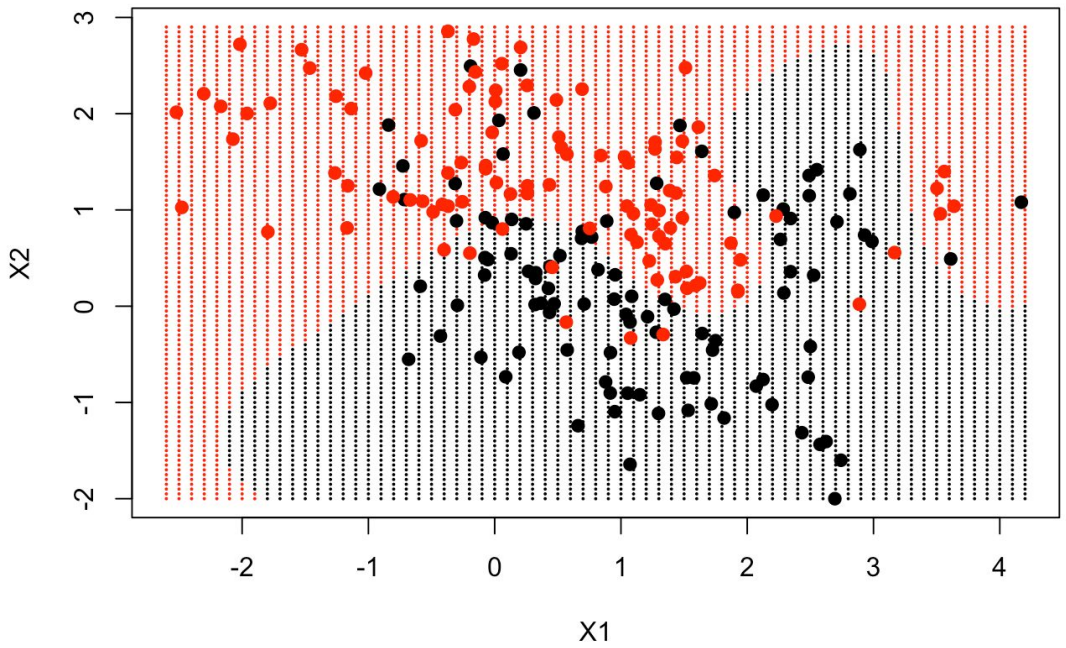
Toaster



Crab (disguised)

# Adversarial examples

- Inevitable consequence of learning in a high-dimensional space?



# Lottery tickets

1. Train a really big network so it works well
2. Prune the trained net so the sparser net works well
3. Go back to the original network at initialization
4. Prune the same weights that you pruned after training
5. Train the pruned net
6. Works just as well or better!

"The lottery ticket hypothesis: finding sparse, trainable neural networks", Frankle and Carbin, ICLR 2019

# Lottery tickets

**The Lottery Ticket Hypothesis.** *A randomly-initialized, dense neural network contains a subnetwork that is initialized such that—when trained in isolation—it can match the test accuracy of the original network after training for at most the same number of iterations.*

- If you knew the right weights to prune in advance, you wouldn't need a massive network
- Suggests that a large network is an ensemble of many subnetworks - one of which got the "golden ticket" in the random initialization

"The lottery ticket hypothesis: finding sparse, trainable neural networks", Frankle and Carbin, ICLR 2019

# The optimization landscape

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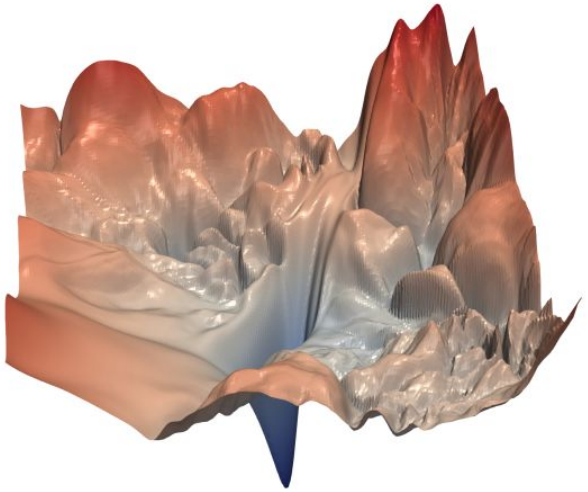
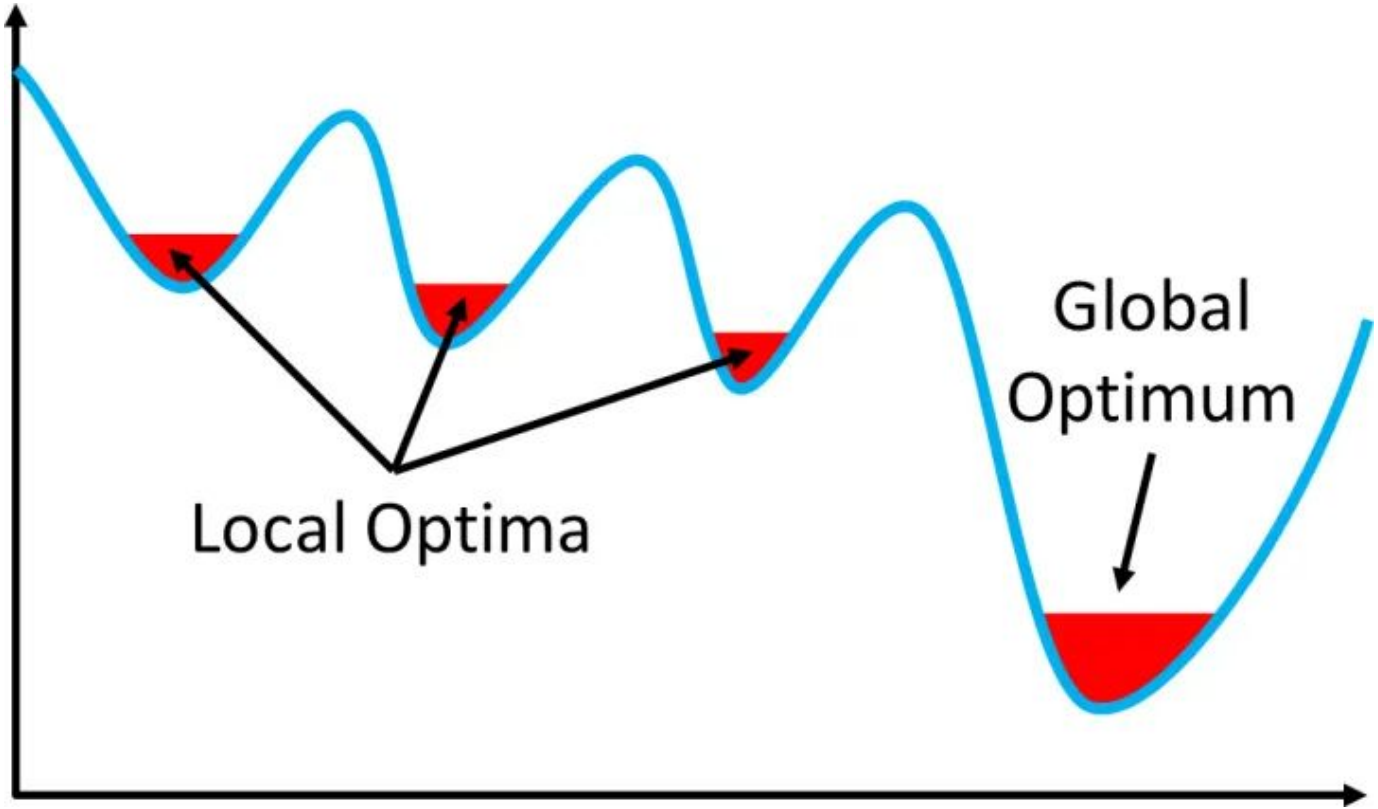
# The optimization landscape

- Shows how the loss varies as you vary the parameters
- Essentially, graph of loss w.r.t. parameters
- So 1M-dimensional if 1M parameters - hard to visualize

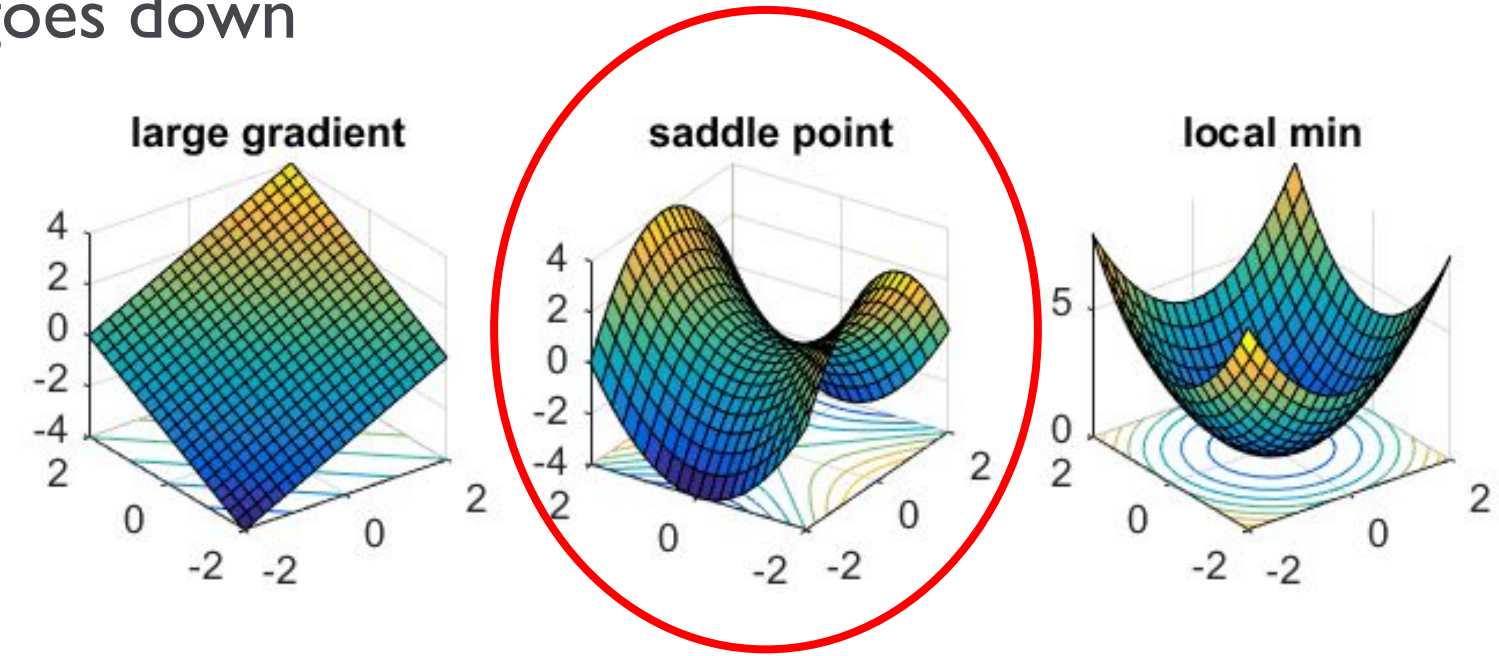


# Local and global optima



# Saddle points

- Some parameter directions, loss goes up, some the loss goes down



# High-dimensional optimization

- Since lots of possible directions, local minima actually generally don't occur for large networks
- Lots of saddle points though

# Real problem: flat areas

- Flat area: most directions the loss stays roughly the same
- Problem because hard to get out of

# Example: XOR

- Input: A set of vectors with 0/1 entries
- Learn: A subset of entries, which are being XORed

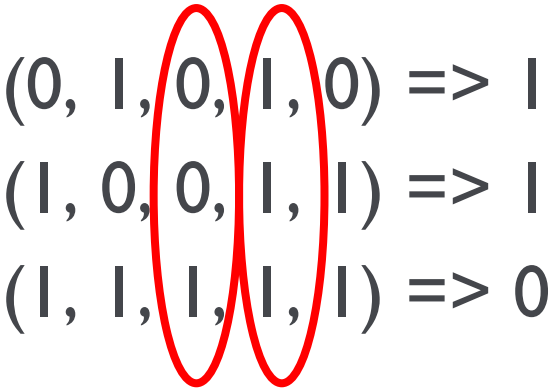
(0, 1, 0, 1, 0) => 1

(1, 0, 0, 1, 1) => 1

(1, 1, 1, 1, 1) => 0

# Example: XOR

- Input: A set of vectors with 0/1 entries
- Learn: A subset of entries, which are being XORed



# Example: XOR

- Input: A set of vectors with 0/1 entries
- Learn: A subset of entries, which are being XORed
- **Provably hard to work out** by gradient descent
- Entire loss landscape is flat except *right around* the global minimum, which is very steep

# How learning rate affects learning

- If learning rate small, more likely to fall into a steep minimum
- Can be good if learning process is hard

# Large learning rate a form of regularization

- Fall into steep minima can be bad for generalization
- The broader, flatter minima may be more robust
- Larger learning rate => can be harder to learn, but better generalization

# Small batch size ⇔ large learning rate

- Small batch size => noisy estimates of gradient
- Also a way to improve generalization
- Increasing the batch size is like decreasing the learning rate
- ½ learning rate can be interpreted as either 2 x batch size or 4 x batch size, depending on perspective

# Second-order methods

- Hessian - second derivatives, capturing curvature:

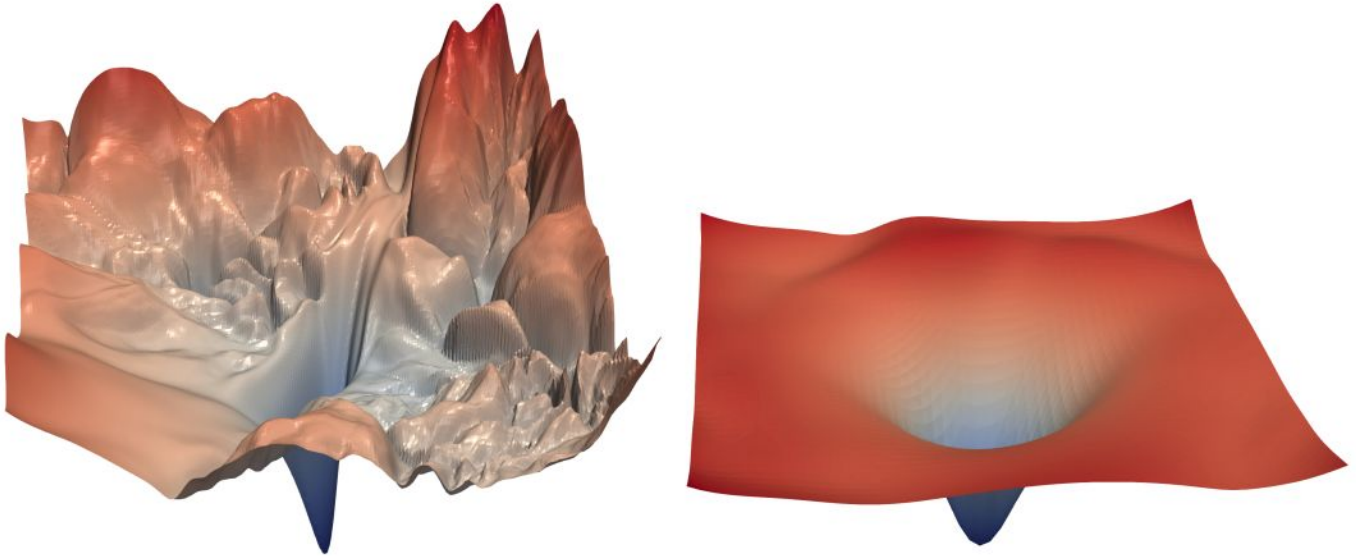
$$H(e) = \begin{bmatrix} \frac{\partial^2 e}{\partial w_1^2} & \frac{\partial^2 e}{\partial w_1 \partial w_2} & \cdots & \frac{\partial^2 e}{\partial w_1 \partial w_n} \\ \frac{\partial^2 e}{\partial w_2 \partial w_1} & \frac{\partial^2 e}{\partial w_2^2} & \cdots & \frac{\partial^2 e}{\partial w_2 \partial w_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 e}{\partial w_n \partial w_1} & \frac{\partial^2 e}{\partial w_n \partial w_2} & \cdots & \frac{\partial^2 e}{\partial w_n^2} \end{bmatrix}$$

# Why not always calculate the Hessian?

# Why not always calculate the Hessian?

- Number of entries is # params squared!
- Too expensive generally
- Some methods approximate the eigenvalues of the Hessian

# Cool picture: ResNet loss landscape



(a) without skip connections

(b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

"Visualizing the loss landscapes of neural nets", Li et al, NeurIPS 2018

# Meta-learning

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# Meta-learning framework

## Training task 1

Support set

K=2

N=3

Query set

## Training task 2 . . .

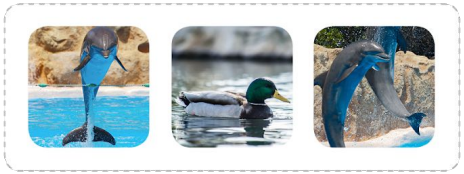
Support set

Query set

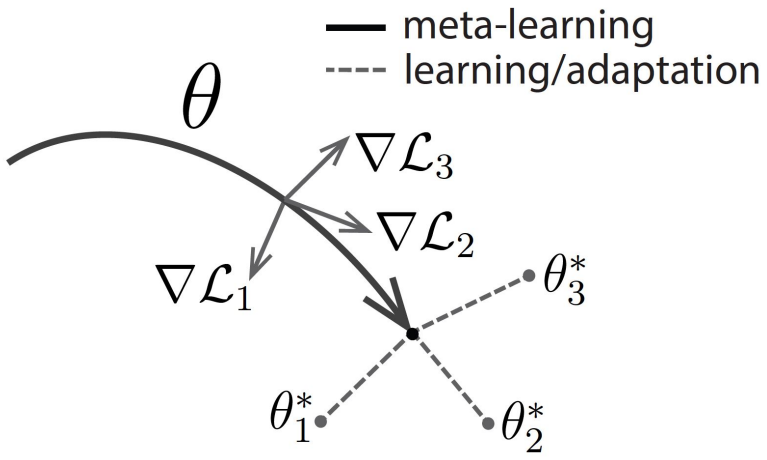
## Test task 1 . . .

Support set

Query set



# Model-agnostic meta-learning (MAML)




**Algorithm 1** Model-Agnostic Meta-Learning

**Require:** $p(\mathcal{T})$: distribution over tasks
**Require:** $\alpha$, $\beta$: step size hyperparameters
1: randomly initialize $\theta$
2: **while** not done **do**
3: Sample batch of tasks $\mathcal{T}_i \sim p(\mathcal{T})$
4: **for all** $\mathcal{T}_i$ **do**
5: Evaluate $\nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$ with respect to $K$ examples
6: Compute adapted parameters with gradient descent: $\theta_i' = \theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$
7: **end for**
8: Update $\theta \leftarrow \theta - \beta \nabla_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$
9: **end while**