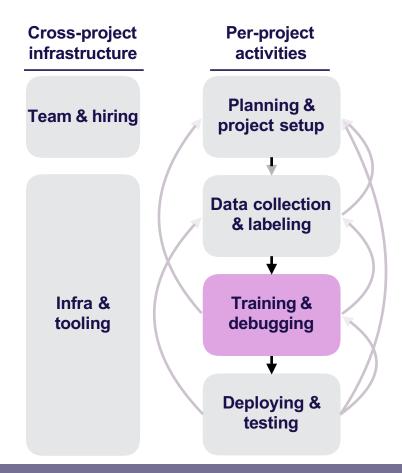


## Troubleshooting Deep Neural Networks

#### Class Annoucement

- HW1 Grading: Released
- HW2 Submission: due Feb 14 (tomorrow)
- HW3: Release next week
- Midterm and Final Exams: Team Projects
- Invited Talk: Walmart (Thu, Feb. 20)

## Lifecycle of a ML project



#### Why talk about DL troubleshooting?



XKCD, https://xkcd.com/1838/

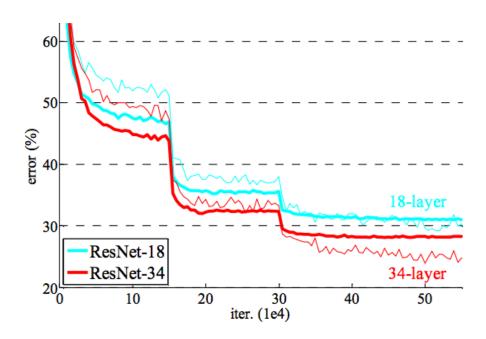
#### Why talk about DL troubleshooting?

#### **Common sentiment among practitioners:**

80-90% of time debugging and tuning

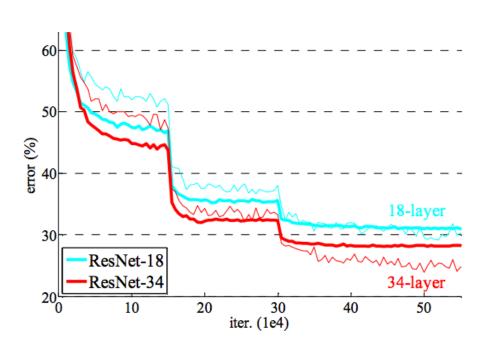
10-20% deriving math or implementing things

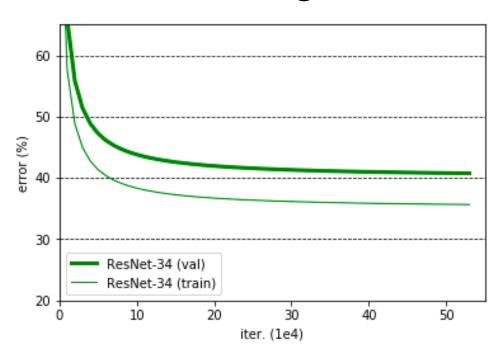
## Why is DL troubleshooting so hard?



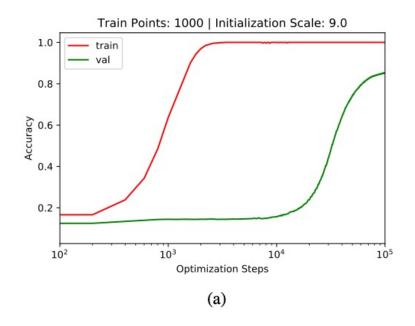
He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.

#### Your learning curve





He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.



https://papers.neurips.cc/paper\_files/paper/2022/file/dfc310e81992d2e4cedc09ac47eff13e-Paper-Conference.pdf

#### **Grokking**

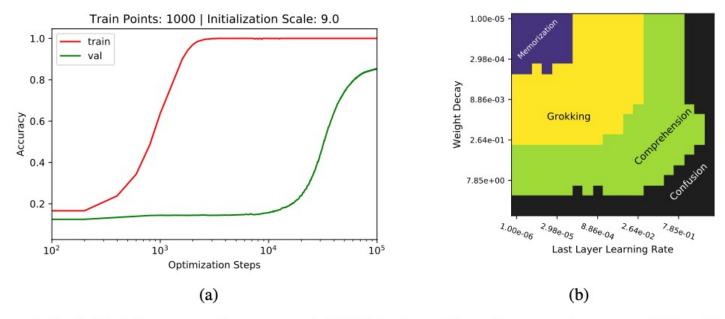


Figure 8: Left: Training curves for a run on MNIST, in the setting where we observe grokking. Right: Phase diagram with the four phases of learning dynamics on MNIST.

#### Towards Understanding Grokking: An Effective Theory of Representation Learning

Ziming Liu, Ouail Kitouni, Niklas Nolte, Eric J. Michaud, Max Tegmark, Mike Williams
Department of Physics, Institute for AI and Fundamental Interactions, MIT
{zmliu,kitouni,nnolte,ericjm,tegmark,mwill}@mit.edu

#### Abstract

We aim to understand grokking, a phenomenon where models generalize long after overfitting their training set. We present both a microscopic analysis anchored by an effective theory and a macroscopic analysis of phase diagrams describing learning performance across hyperparameters. We find that generalization originates from structured representations whose training dynamics and dependence on training set size can be predicted by our effective theory in a toy setting. We observe empirically the presence of four learning phases: comprehension, grokking, memorization, and confusion. We find representation learning to occur only in a "Goldilocks zone" (including comprehension and grokking) between memorization and confusion. We find on transformers the grokking phase stays closer to the memorization phase (compared to the comprehension phase), leading to delayed generalization. The Goldilocks phase is reminiscent of "intelligence from starvation" in Darwinian evolution, where resource limitations drive discovery of more efficient solutions. This study not only provides intuitive explanations of the origin of grokking, but also highlights the usefulness of physics-inspired tools, e.g., effective theories and phase diagrams, for understanding deep learning.

Poor model performance

Implementation bugs

Poor model performance

## Most DL bugs are invisible

```
features = glob.glob('path/to/features/*')
labels = glob.glob('path/to/labels/*')
train(features, labels)
```



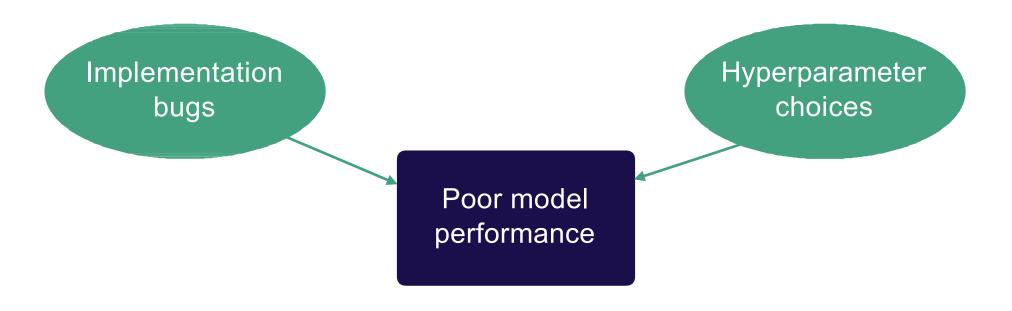
#### Most DL bugs are invisible

# 1 features = glob.glob('path/to/features/\*') 2 labels = glob.glob('path/to/labels/\*') 3 train(features, labels)

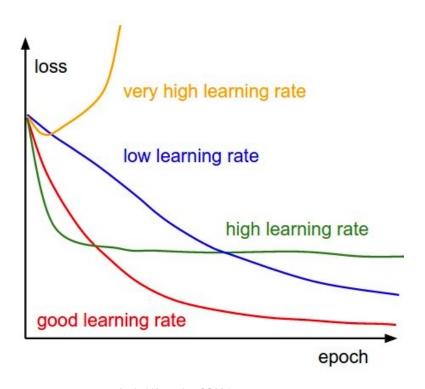


Implementation bugs

Poor model performance

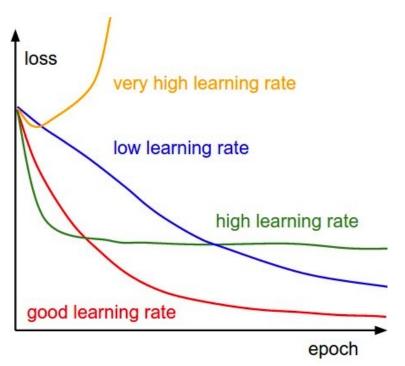


#### Models are sensitive to hyperparameters

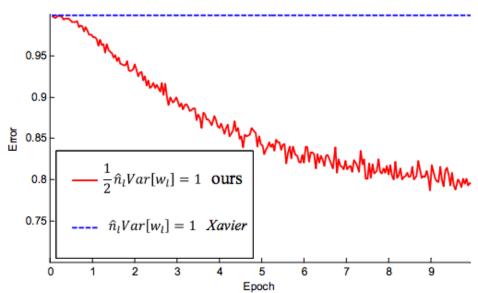


Andrej Karpathy, CS231n course notes

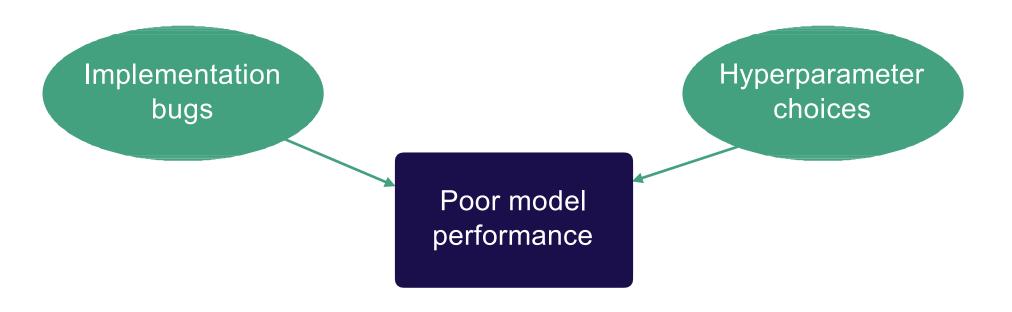
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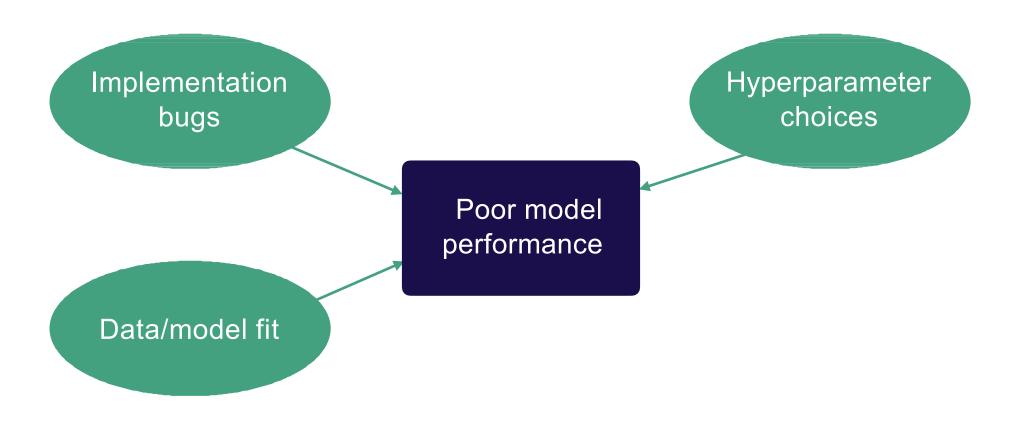


Andrej Karpathy, CS231n course notes



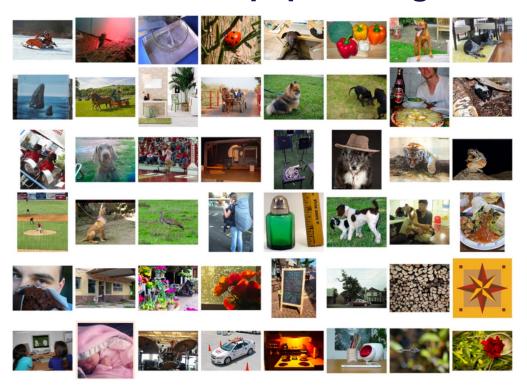
He, Kaiming, et al. "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification." Proceedings of the IEEE international conference on computer vision. 2015.





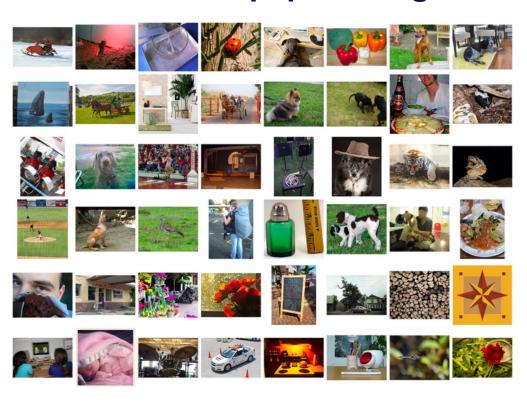
#### Data / model fit

#### Data from the paper: ImageNet



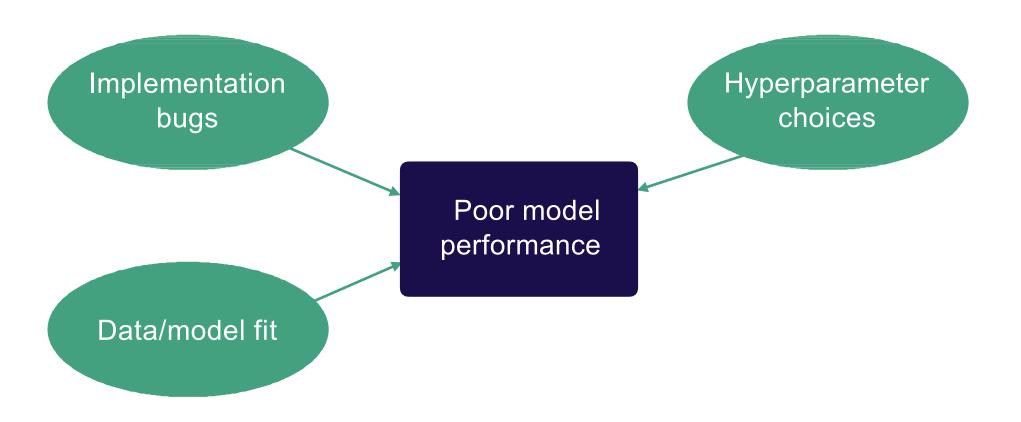
#### Data / model fit

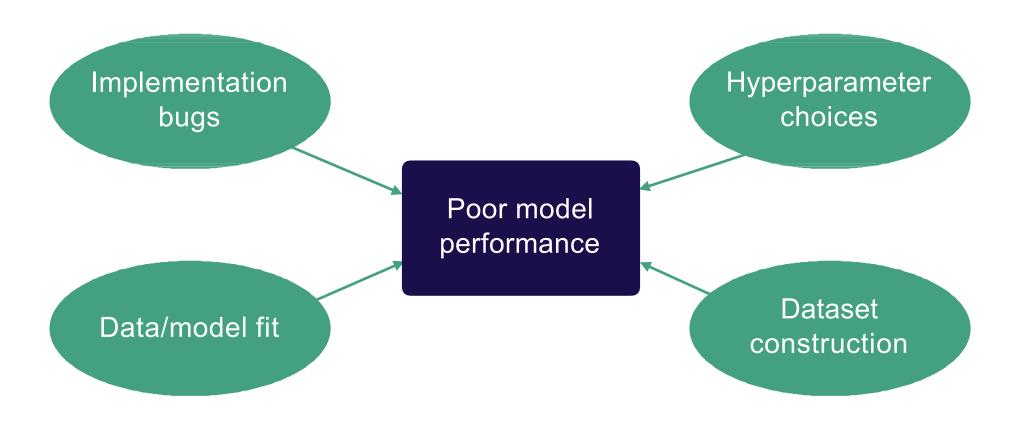
#### **Data from the paper: ImageNet**



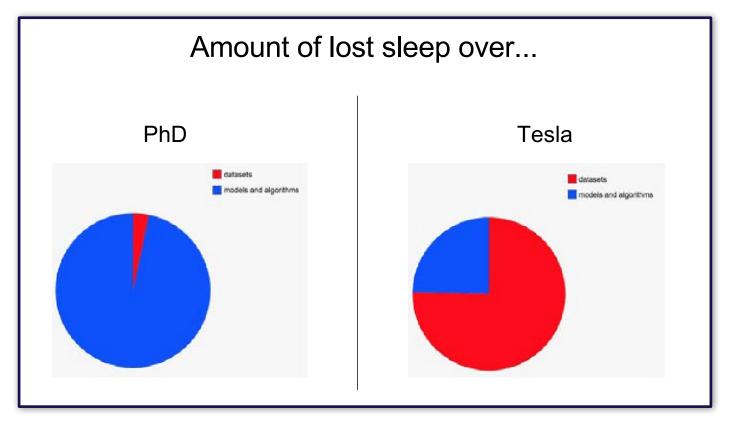
#### Yours: self-driving car images







#### Constructing good datasets is hard



Slide from Andrej Karpathy's talk "Building the Software 2.0 Stack" at TrainAl 2018, 5/10/2018

#### Common dataset construction issues

- Not enough data
- Class imbalances
- Noisy labels
- Train / test from different distributions
- etc

#### Takeaways: why is troubleshooting hard?

- Hard to tell if you have a bug
- Lots of possible sources for the same degradation in performance
- Results can be sensitive to small changes in hyperparameters and dataset makeup

## Strategy for DL troubleshooting

## Key mindset for DL troubleshooting

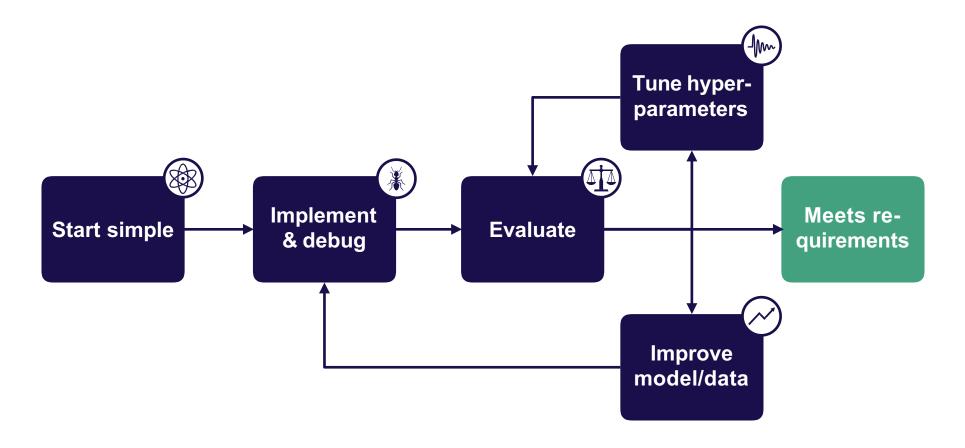
#### **Pessimism**

#### Key idea of DL troubleshooting

Since it's hard to disambiguate errors...

...Start simple and gradually ramp up complexity

#### Strategy for DL troubleshooting





 Choose the simplest model & data possible (e.g., LeNet on a subset of your data)



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Once model runs, overfit a single batch & reproduce a known result



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 Apply the bias-variance decomposition to decide what to do next



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## Quick summary



 Choose the simplest model & data possible (e.g., LeNet on a subset of your data)



Once model runs, overfit a single batch & reproduce a known result



 Apply the bias-variance decomposition to decide what to do next



Use coarse-to-fine random searches



 Make your model bigger if you underfit; add data or regularize if you overfit

# We'll assume you already have...

- Initial test set
- A single metric to improve
- Target performance based on human-level performance, published results, previous baselines, etc

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- Target performance based on human-level performance, published results, previous baselines, etc

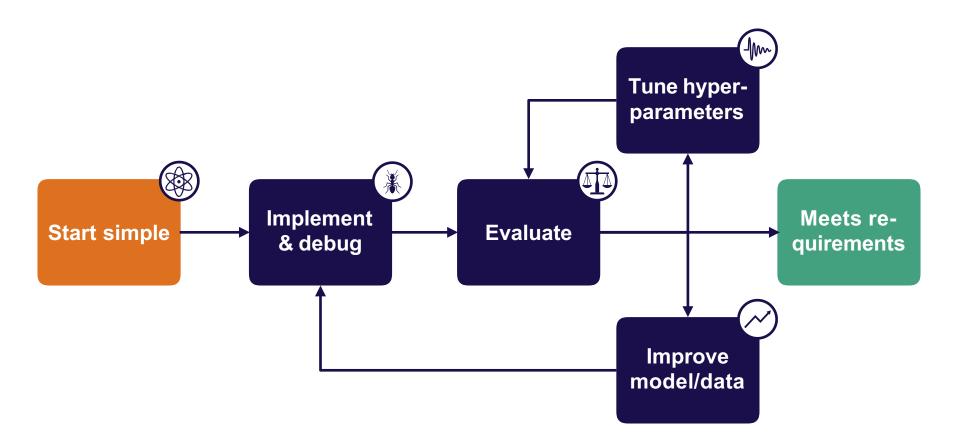
#### **Running example**



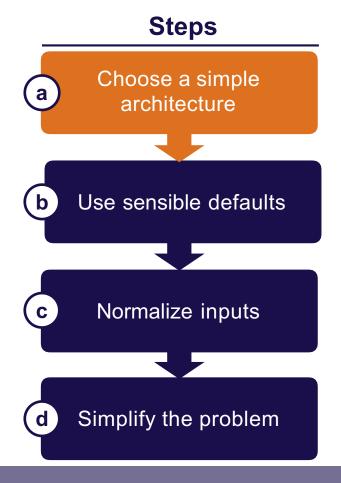
**Goal:** 99% classification accuracy

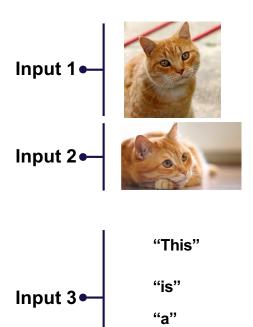
# Questions?

## Strategy for DL troubleshooting

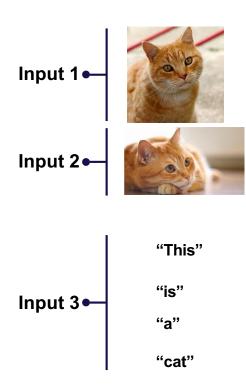


# Starting simple

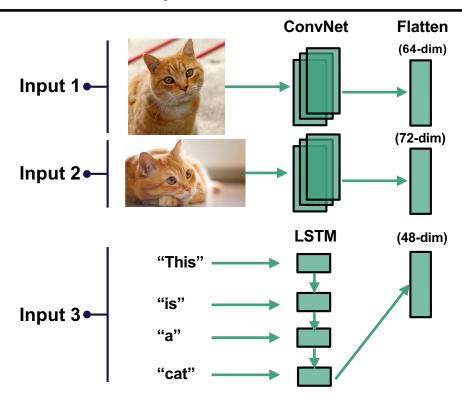




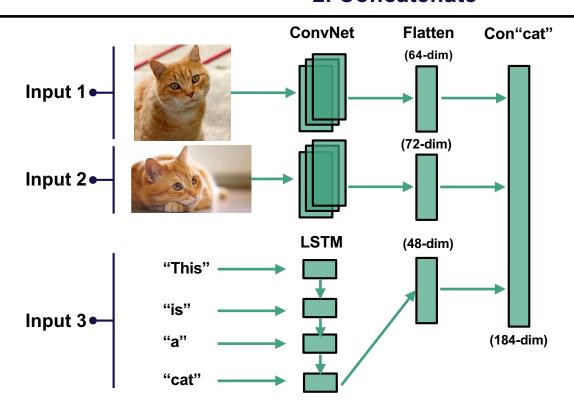
#### 1. Map each into a lower dimensional feature space



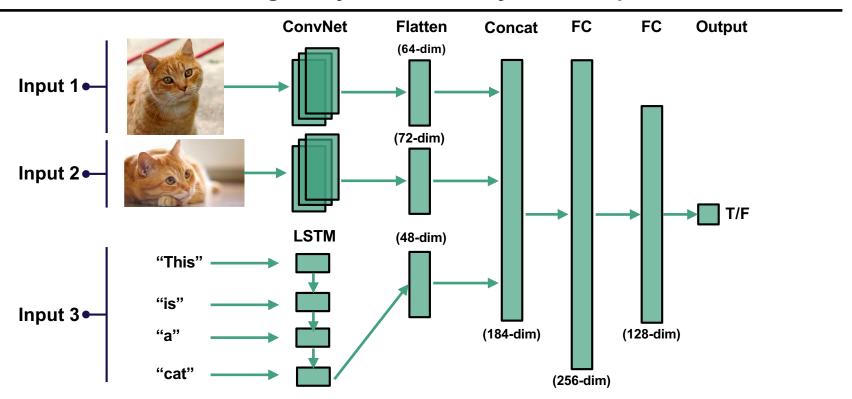
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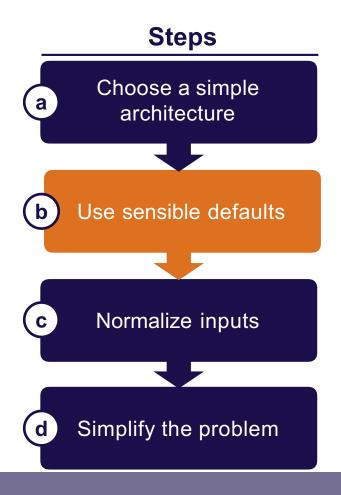
#### 2. Concatenate



#### 3. Pass through fully connected layers to output



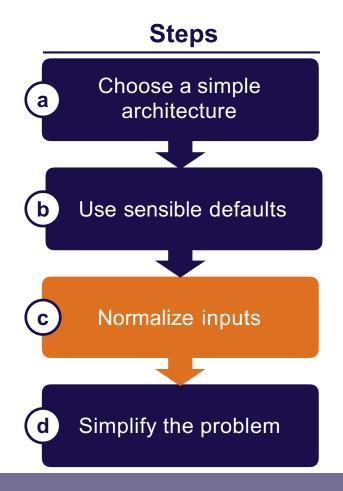
# Starting simple



#### Recommended network / optimizer defaults

- Optimizer: Adam optimizer with learning rate 3e-4
- Activations: relu (FC and Conv models), tanh (LSTMs)
- Initialization: He et al. normal (relu), Glorot normal (tanh)
- Regularization: None
- Data normalization: None

# Starting simple

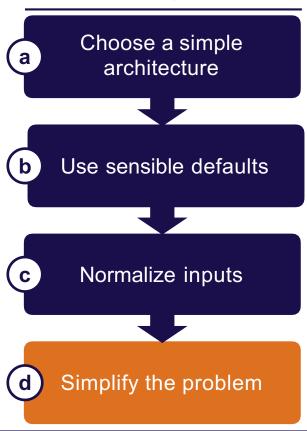


#### Important to normalize scale of input data

- Subtract mean and divide by variance
- For images, fine to scale values to [0, 1] or [-0.5, 0.5] (e.g., by dividing by 255) [Careful, make sure your library doesn't do it for you!]

# Starting simple

#### **Steps**



## Consider simplifying the problem as well

- Start with a small training set (~10,000 examples)
- Use a fixed number of objects, classes, image size, etc.
- Create a simpler synthetic training set

## Simplest model for pedestrian detection

- Start with a subset of 10,000 images for training, 1,000 for val, and 500 for test
- Use a LeNet architecture with sigmoid cross-entropy loss
- Adam optimizer with LR 3e-4
- No regularization

#### Simplest model for pedestrian detection

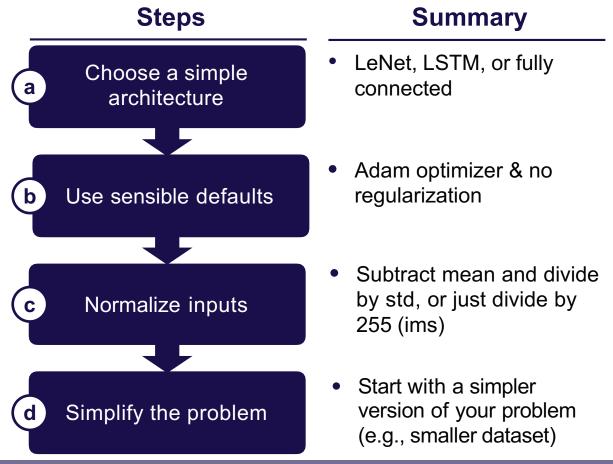
#### Running example

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Goal: 99% classification accuracy

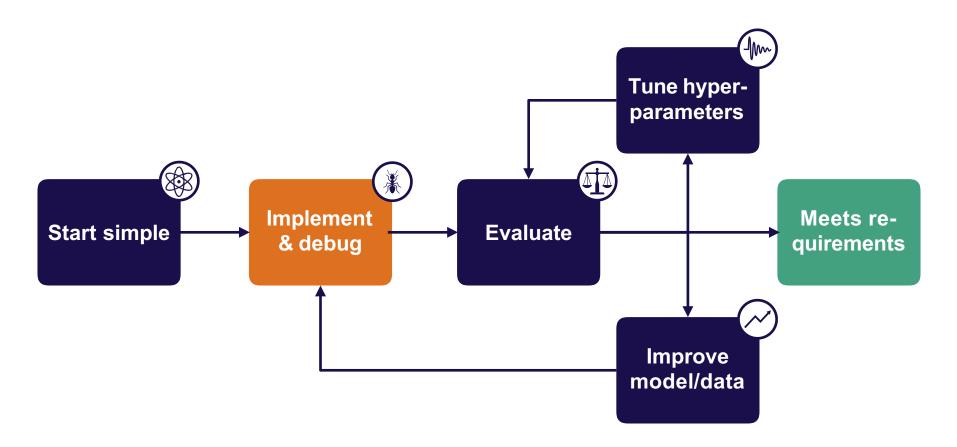
## Starting simple

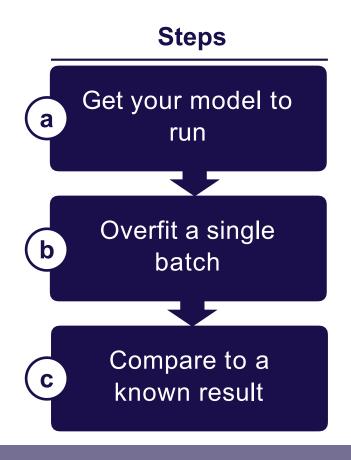


Questions?



## Strategy for DL troubleshooting





Incorrect shapes for your tensors

Can fail silently! E.g., accidental broadcasting: x.shape = (None,), y.shape = (None, 1), (x+y).shape = (None, None)

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- Forgot to set up train mode for the net correctly
   E.g., toggling train/eval, controlling batch norm dependencies
- Numerical instability inf/NaN
   Often stems from using an exp, log, or div operation

#### General advice for implementing your model

#### **Lightweight implementation**

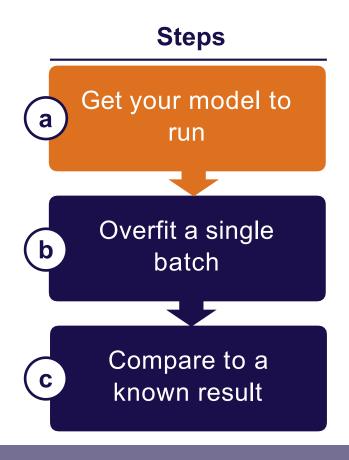
- Minimum possible new lines of code for v1
- Rule of thumb: <200 lines</li>
- (Tested infrastructure components are fine)

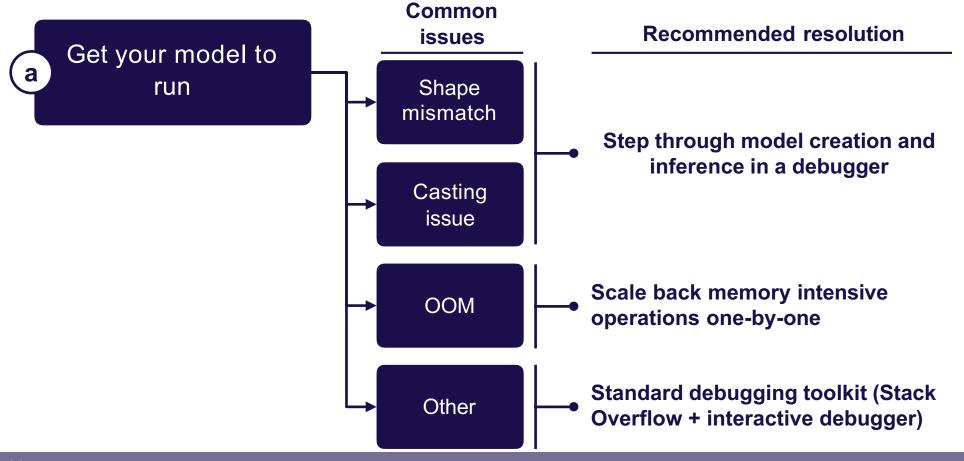
#### Use off-the-shelf components, e.g.,

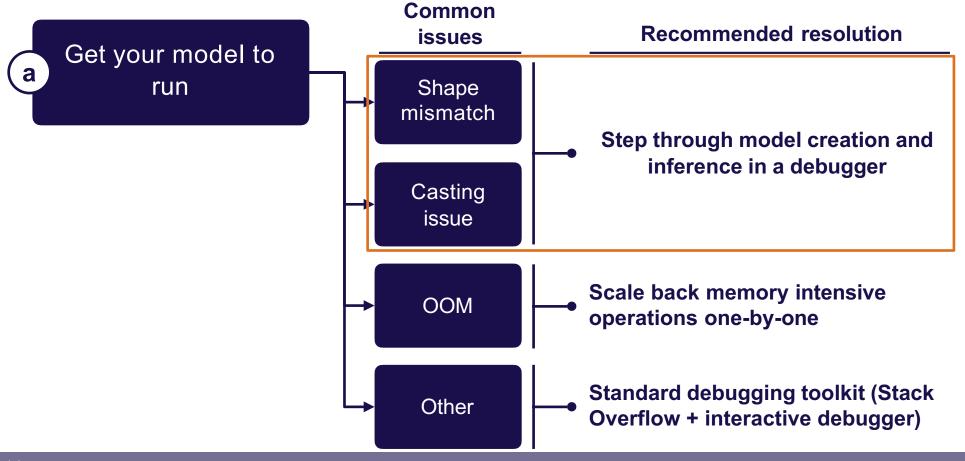
- Keras
- tf.layers.dense(...)
   instead of
   tf.nn.relu(tf.matmul(W, x))
- tf.losses.cross\_entropy(...) instead of writing out the exp

#### **Build complicated data pipelines later**

 Start with a dataset you can load into memory







## Debuggers for DL code

- Pytorch: easy, use ipdb
- tensorflow: trickier

#### **Option 1: step through graph creation**

```
2 # Option 1: step through graph creation
3 import ipdb; ipdb.set_trace()
4
5 for i in range(num_layers):
6     out = layers.fully_connected(out, 50)
7
```

## Debuggers for DL code

- Pytorch: easy, use ipdb
- tensorflow: trickier

#### **Option 2: step into training loop**

```
9 # Option 2: step into training loop
10 sess = tf.Session()
11 for i in range(num_epochs):
12    import ipdb; ipdb.set_trace()
13    loss_, _ = sess.run([loss, train_op])
14
```

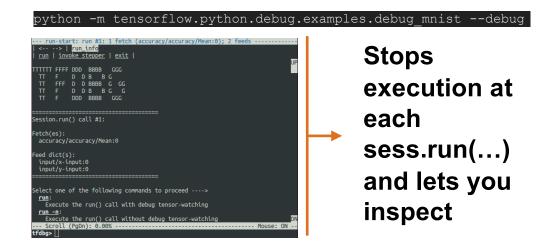
**Evaluate tensors using sess.run(...)** 

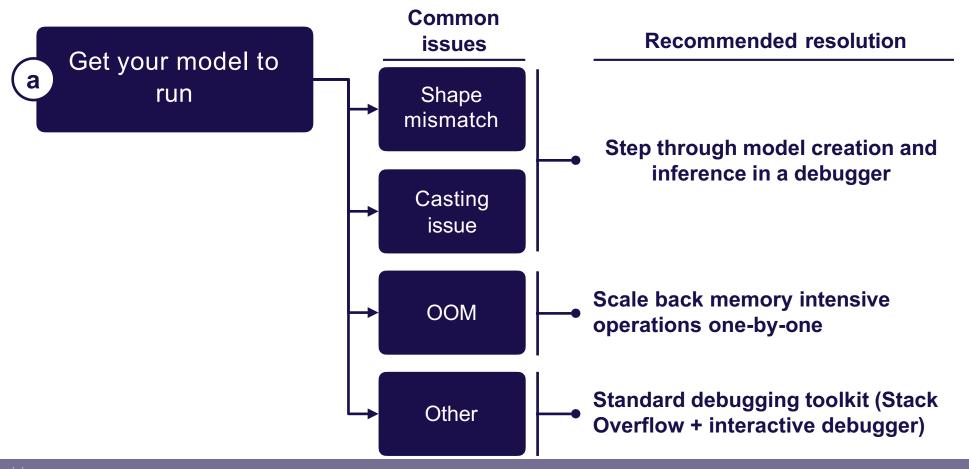
# Debuggers for DL code

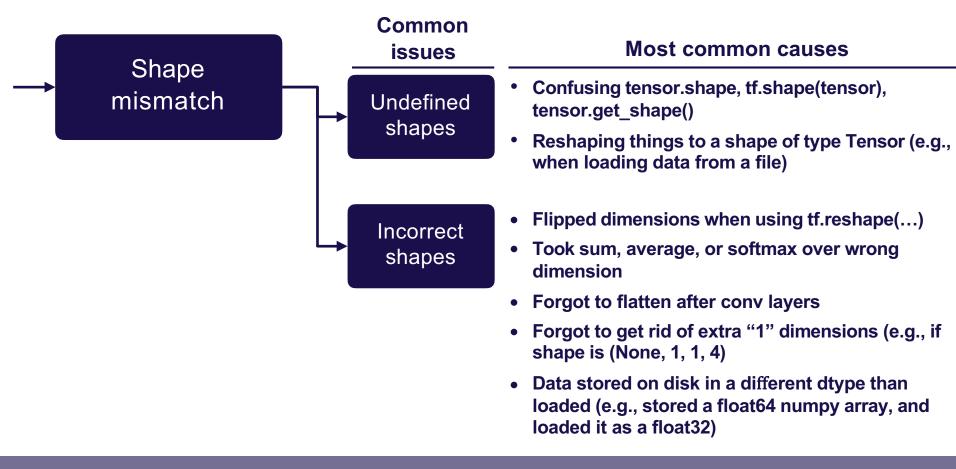
Pytorch: easy, use ipdb

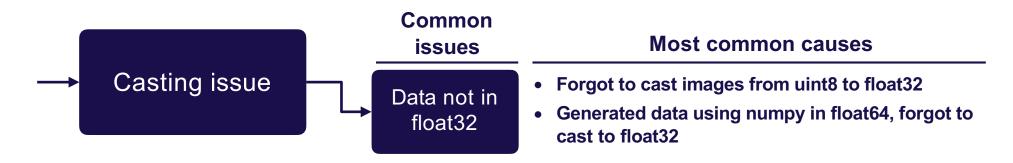
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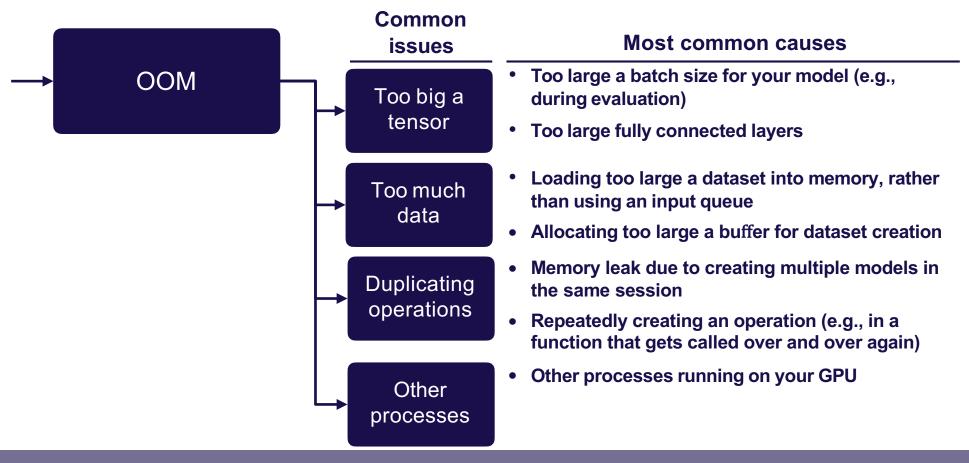
#### Option 3: use tfdb

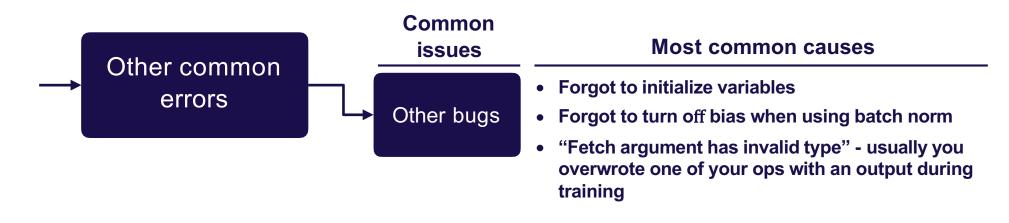


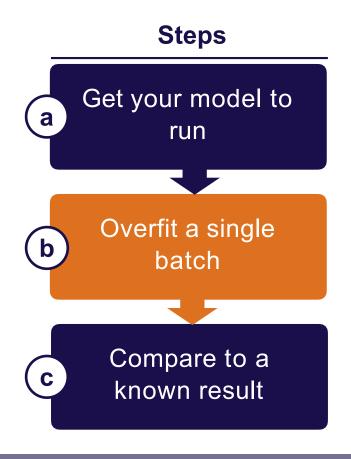


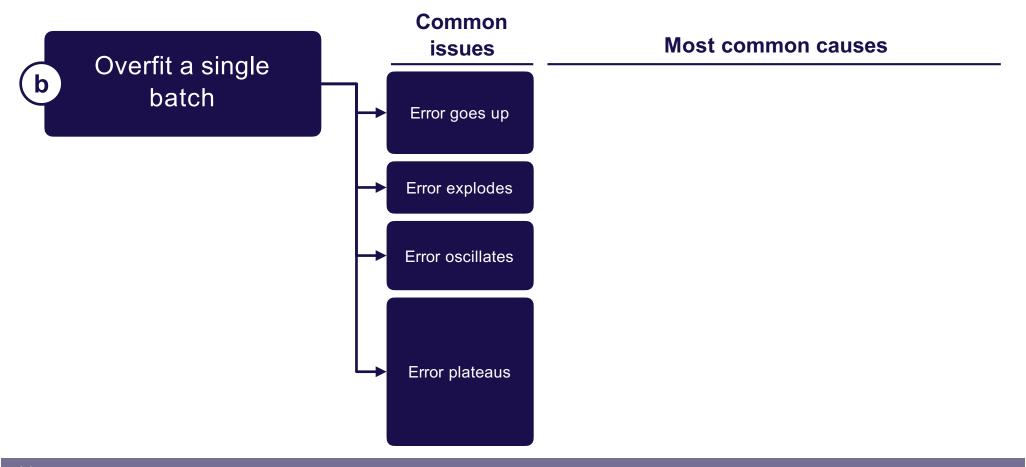


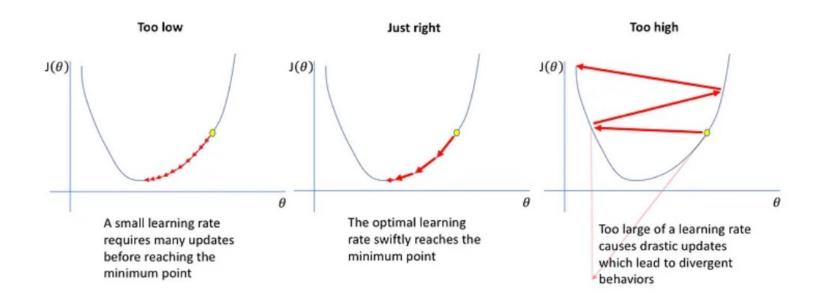






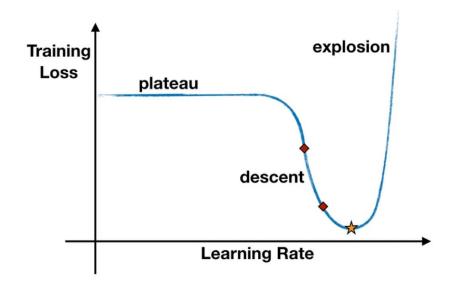




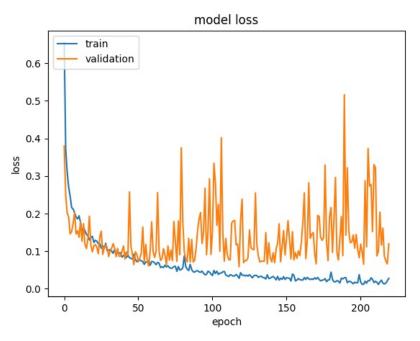


https://medium.com/data-from-the-trenches/the-learning-rate-black-magic-c4a652133cd7



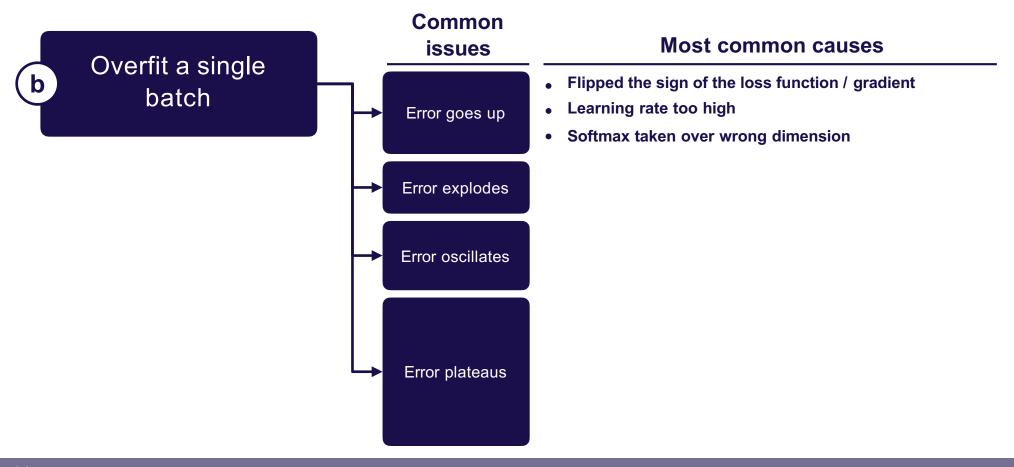


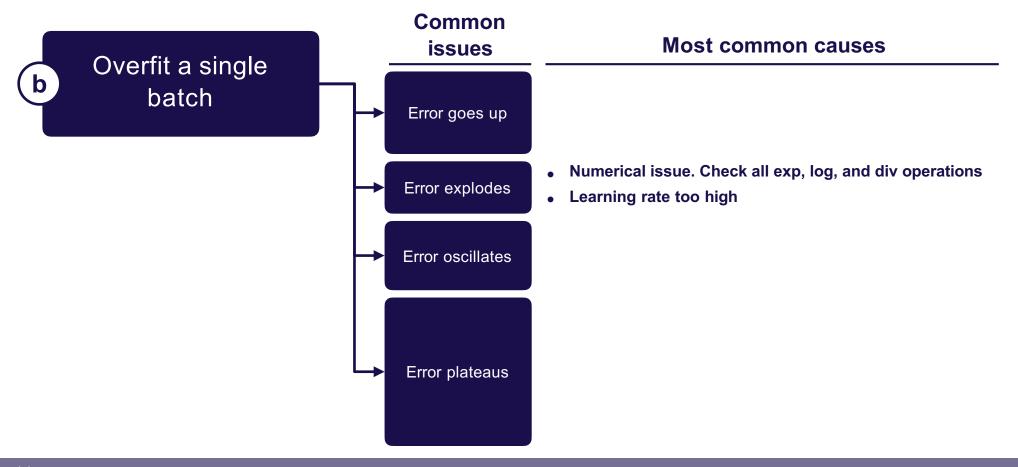
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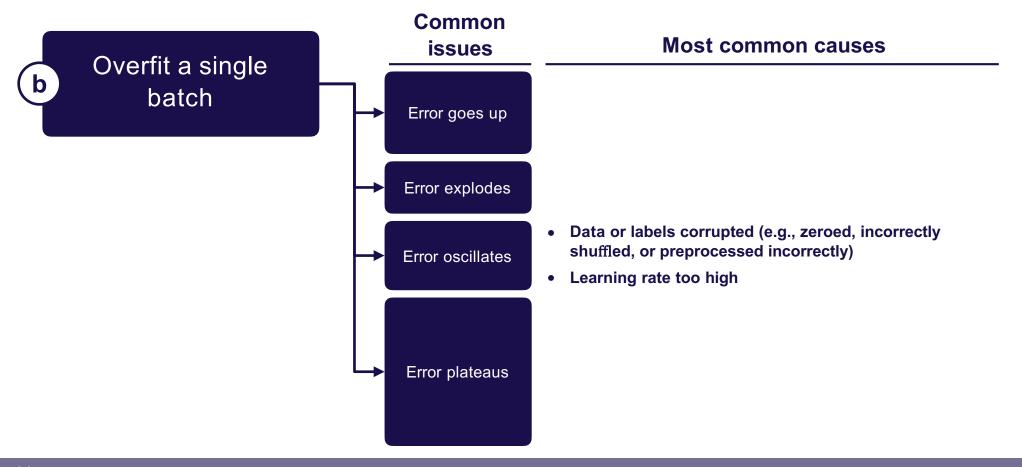


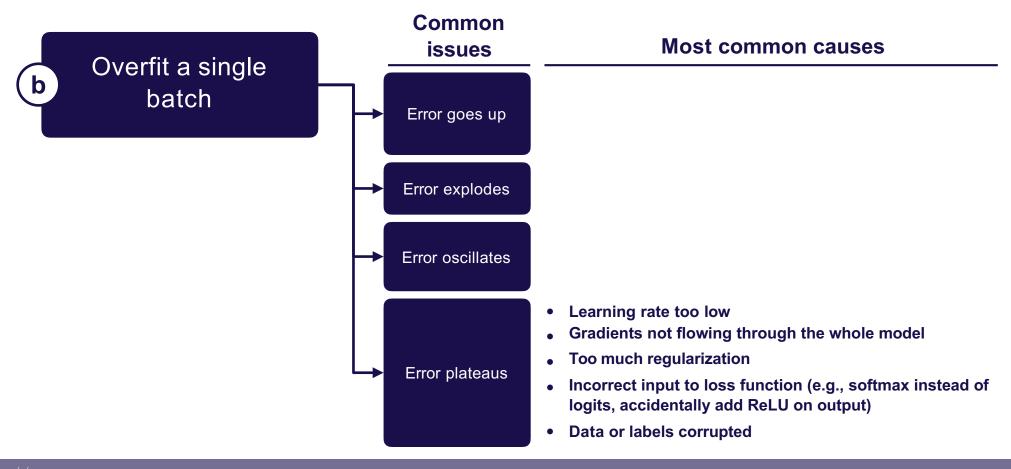
**Error oscillates** 

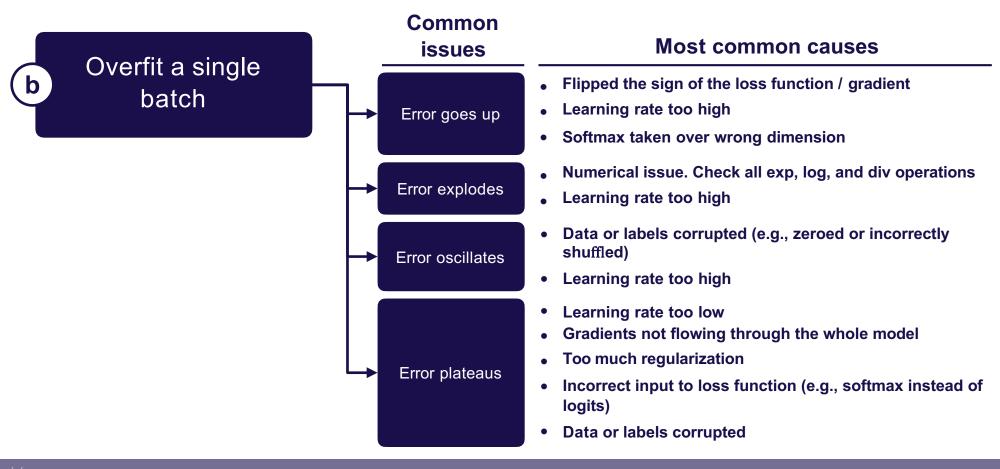
https://medium.com/data-from-the-trenches/the-learning-rate-black-magic-c4a652133cd7

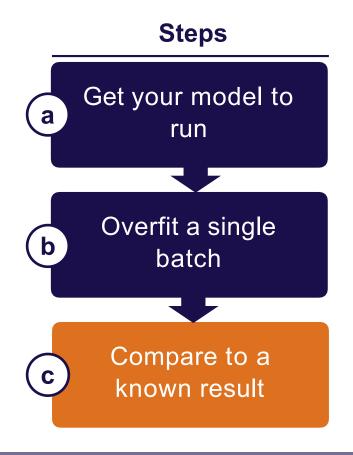












# More useful

 Official model implementation evaluated on similar dataset to yours

#### You can:

- Walk through code line-by-line and ensure you have the same output
- Ensure your performance is up to par with expectations

# More useful

 Official model implementation evaluated on benchmark (e.g., MNIST)

#### You can:

 Walk through code line-by-line and ensure you have the same output

# More useful

Unofficial model implementation

#### You can:

• Same as before, but with lower confidence

# More useful

Results from a paper (with no code)

#### You can:

Ensure your performance is up to par with expectations

# More useful

#### You can:

- Make sure your model performs well in a simpler setting
- Results from your model on a benchmark dataset (e.g., MNIST)

# More useful

#### You can:

 Get a general sense of what kind of performance can be expected

· Results from a similar model on a similar dataset

# More useful

#### You can:

 Make sure your model is learning anything at all

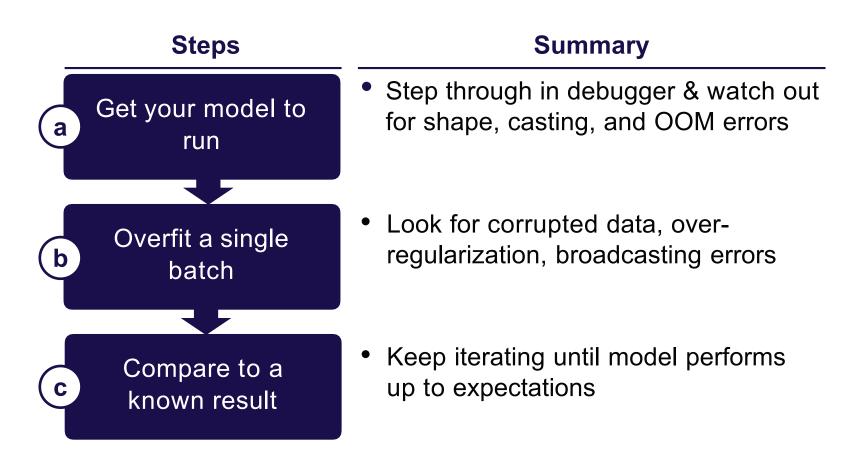
#### Less useful

• Super simple baselines (e.g., average of outputs or linear regression)

# More useful

- Official model implementation evaluated on similar dataset to yours
- Official model implementation evaluated on benchmark (e.g., MNIST)
- Unofficial model implementation
- Results from the paper (with no code)
- Results from your model on a benchmark dataset (e.g., MNIST)
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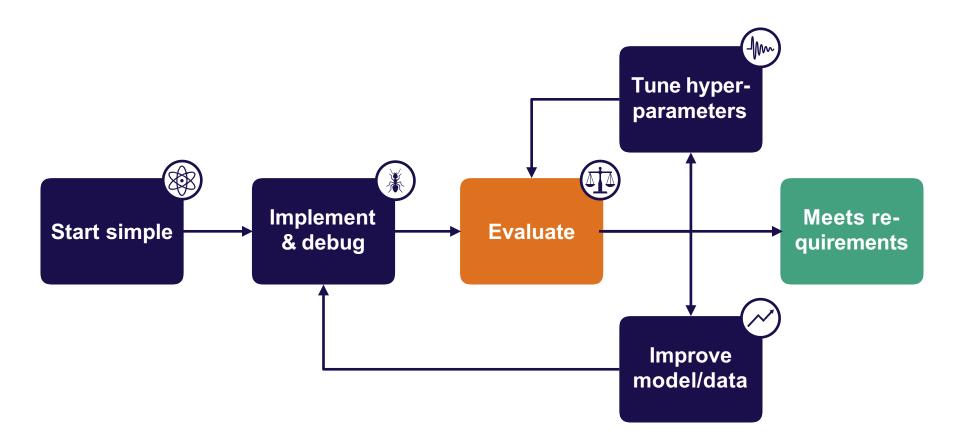
### Summary: how to implement & debug

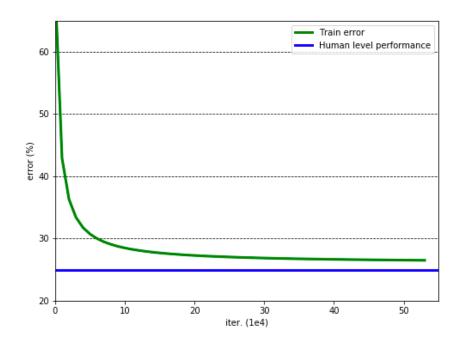


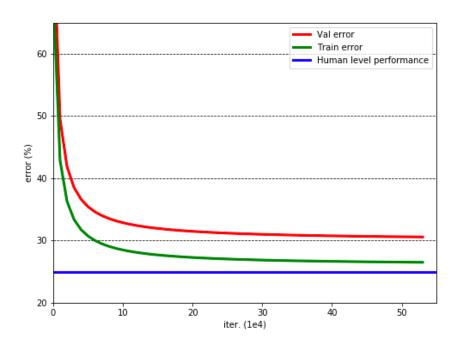
## Questions?

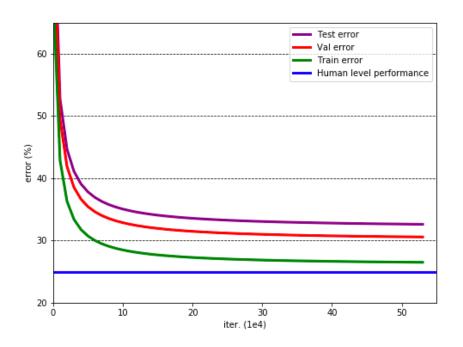


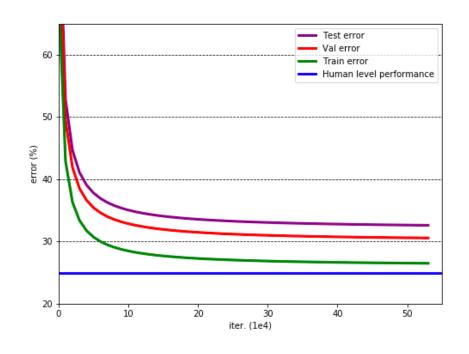
## Strategy for DL troubleshooting

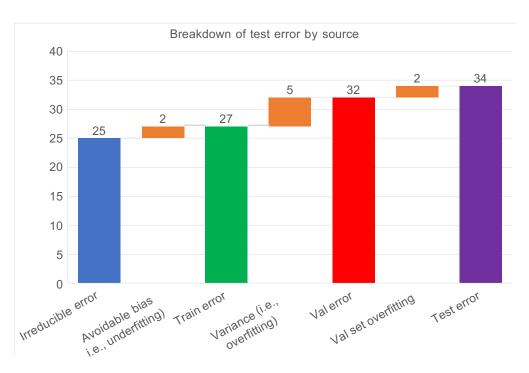












- Test error = irreducible error + bias + variance + val overfitting
- This assumes train, val, and test all come from the same distribution.
   What if not?

## Handling distribution shift

**Train data** 

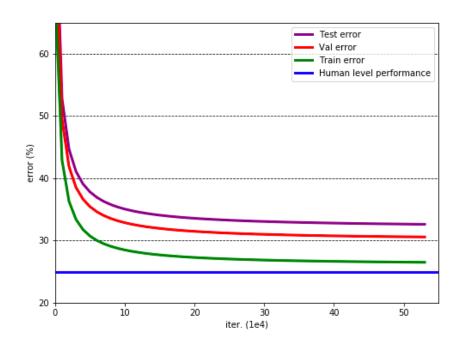


**Test data** 

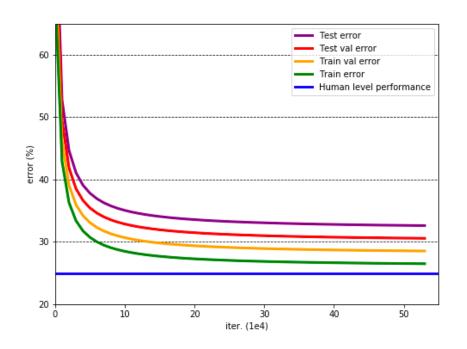


Use two val sets: one sampled from training distribution and one from test distribution

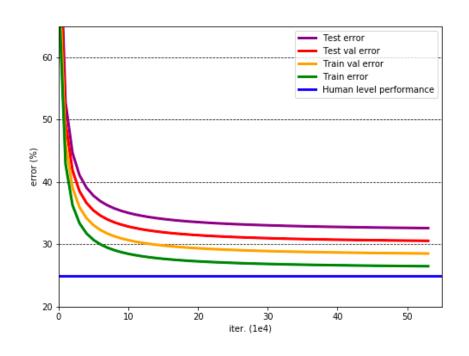
#### The bias-variance tradeoff

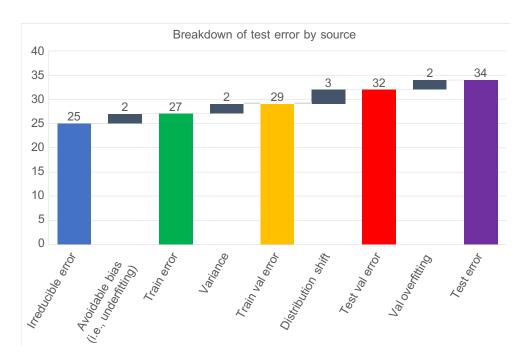


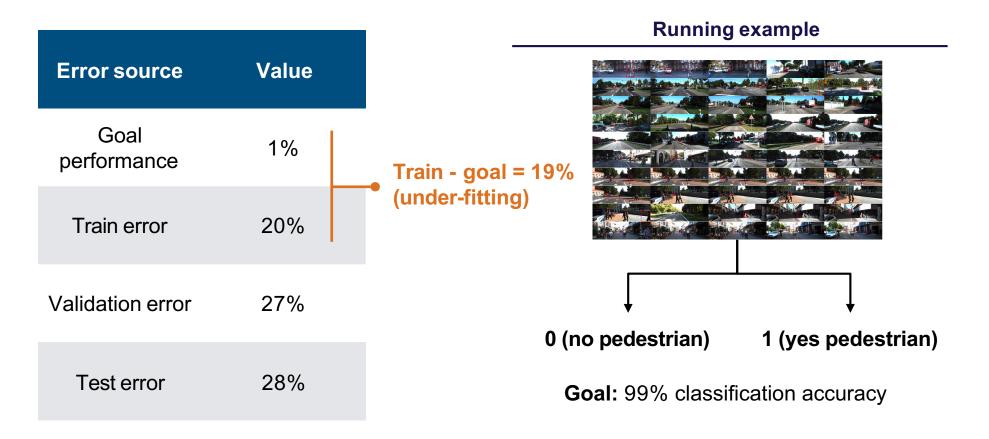
#### Bias-variance with distribution shift



#### Bias-variance with distribution shift







		Running example
Error source	Value	
Goal performance	1%	
Train error	20%	Val - train = 7%
Validation error	27%	(over-fitting)  0 (no pedestrian)  1 (yes pedestrian)
Test error	28%	Goal: 99% classification accuracy

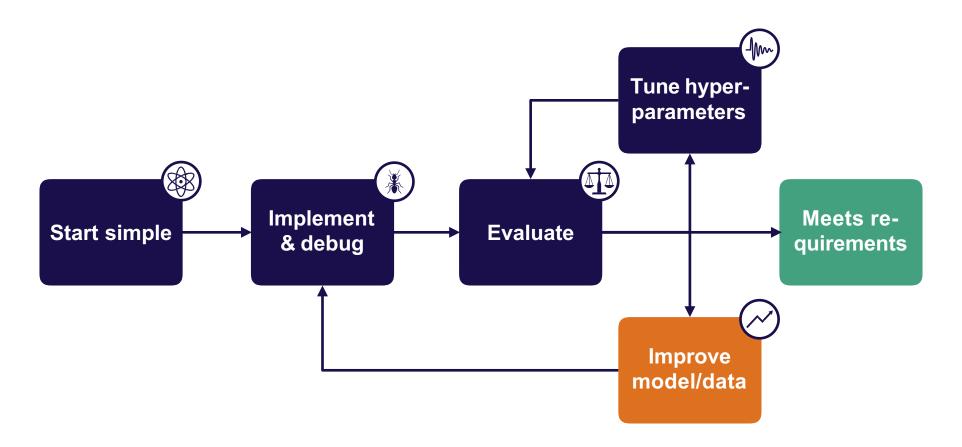
		Running example
Error source	Value	
Goal performance	1%	
Train error	20%	
Validation error	27%	Test - val = 1% 0 (no pedestrian) 1 (yes pedestrian)
Test error	28%	Test - val = 1% (looks good!) 0 (no pedestrian) 1 (yes pedestrian)  Goal: 99% classification accuracy

# Summary: evaluating model performance

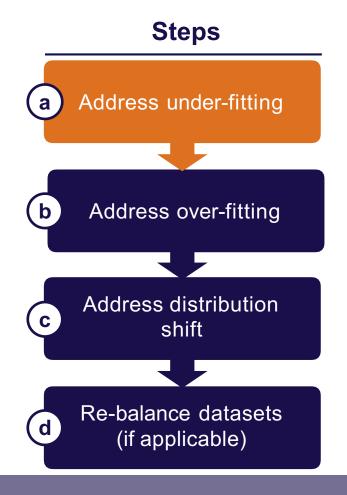
Test error = irreducible error + bias + variance + distribution shift + val overfitting

# Questions?

# Strategy for DL troubleshooting



## Prioritizing improvements (i.e., applied b-v)



## Addressing under-fitting (i.e., reducing bias)

#### Try first

- A. Make your model bigger (i.e., add layers or use more units per layer)
- B. Reduce regularization
- C. Error analysis
- D. Choose a different (closer to state-of-the art) model architecture (e.g., move from LeNet to ResNet)
- E. Tune hyper-parameters (e.g., learning rate)

#### Try later

F. Add features

Add more layers to the ConvNet

Error source	Value	Value
Goal performance	<del>1%</del>	1%
Train error	<del>20%</del>	7%
Validation error	<del>27%</del>	19%
Test error	<del>28%</del>	20%



**Goal:** 99% classification accuracy (i.e., 1% error)

Switch to ResNet-101

Error source	Value	Value	Value
Goal performance	<del>1%</del>	<del>1%</del>	1%
Train error	20%	<del>7%</del>	3%
Validation error	<del>27%</del>	<del>19%</del>	10%
Test error	<del>28%</del>	<del>20%</del>	10%



**Goal:** 99% classification accuracy (i.e., 1% error)

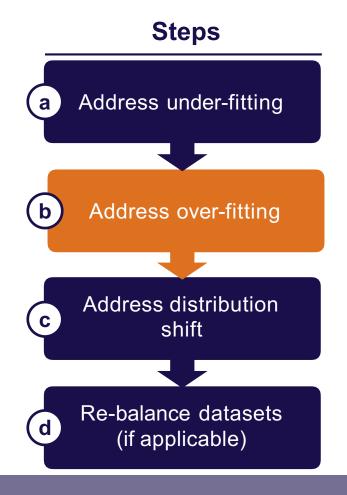
Tune	learning
rate	

Error source	Value	Value	Value	Value
Goal performance	<del>1%</del>	<del>1%</del>	<del>1%</del>	1%
Train error	20%	<del>7%</del>	3%	0.8%
Validation error	<del>27%</del>	<del>19%</del>	<del>10%</del>	12%
Test error	<del>28%</del>	<del>20%</del>	<del>10%</del>	12%



**Goal:** 99% classification accuracy (i.e., 1% error)

## Prioritizing improvements (i.e., applied b-v)



## Addressing over-fitting (i.e., reducing variance)

#### Try first

- A. Add more training data (if possible!)
- B. Add normalization (e.g., batch norm, layer norm)
- C. Add data augmentation
- D. Increase regularization (e.g., dropout, L2, weight decay)
- E. Error analysis
- F. Choose a different (closer to state-of-the-art) model architecture
- G. Tune hyperparameters
- H. Early stopping
- Remove features
- J. Reduce model size

#### **Try later**

## Addressing over-fitting (i.e., reducing variance)

#### Try first

- A. Add more training data (if possible!)
- B. Add normalization (e.g., batch norm, layer norm)
- C. Add data augmentation
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- G. Tune hyperparameters

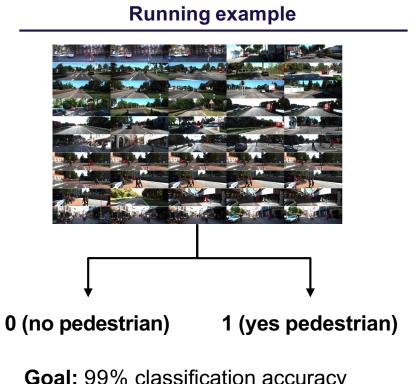
#### H. Early stopping

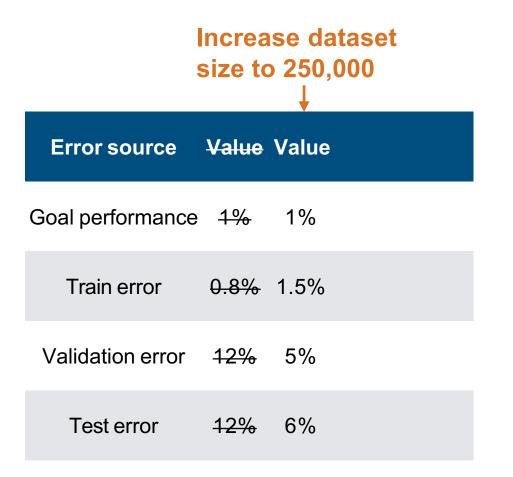
- . Remove features
- J. Reduce model size

#### **Try later**

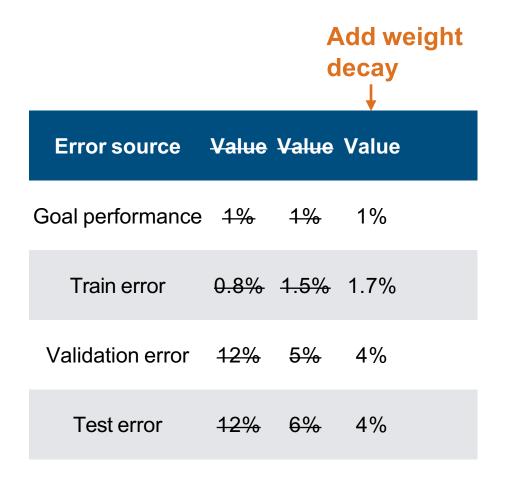
⊓NOT Frecommended!

Error source	Value
Goal performance	1%
Train error	0.8%
Validation error	12%
Test error	12%





# Running example 0 (no pedestrian) 1 (yes pedestrian)



# Running example O (no pedestrian) 1 (yes pedestrian)

Add data augmentation Running example Value Value Value Value **Error source** Goal performance 1% 1% 0.8% 1.5% 1.7% Train error 2% Validation error 12% <del>5%</del> <del>4%</del> 2.5% 0 (no pedestrian) 1 (yes pedestrian) <del>12%</del> <del>6%</del> <del>4%</del> 2.6% Test error Goal: 99% classification accuracy

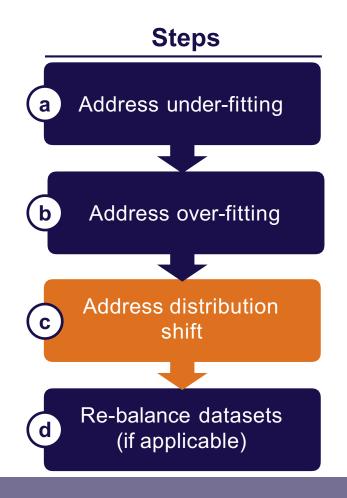
Tune num layers, optimizer params, weight

initialization, kernel size, weight decay

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					<b>*</b>	The state of the s	
Error source	<b>Value</b>	<del>Value</del>	<del>Value</del>	<b>Value</b>	Value		
Goal performance	<del>1%</del>	<del>1%</del>	<del>1%</del>	<del>1%</del>	1%		tun V
Train error	0.8%	<del>1.5%</del>	<del>1.7%</del>	2%	0.6%		
Validation error	<del>12%</del>	<del>5%</del>	<del>4%</del>	<del>2.5%</del>	0.9%	↓ ) (no pedestrian) 1 (y	↓ /es pedestrian)
Test error	<del>12%</del>	<del>6%</del>	4%	<del>2.6%</del>	1.0%	Goal: 99% classification	ı accuracy

## Prioritizing improvements (i.e., applied b-v)



# Addressing distribution shift

#### **Try first**

- A. Analyze test-val set errors & collect more training data to compensate
- B. Analyze test-val set errors & synthesize more training data to compensate
- C. Apply domain adaptation techniques to training & test distributions

**Try later** 

#### Test-val set errors (no pedestrian detected)

















Test-val set errors (no pedestrian detected)

Train-val set errors (no pedestrian detected)















Error type 1: hard-to-see pedestrians

Test-val set errors (no pedestrian detected)

Train-val set errors (no pedestrian detected)















**Error type 2:** reflections

Test-val set errors (no pedestrian detected)

Train-val set errors (no pedestrian detected)















Error type 3 (test-val only): night scenes

Error type	Error % (train-val)	Error % (test-val)	Potential solutions	Priority
Hard-to-see     pedestrians	0.1%	0.1%	Better sensors	Low
2. Reflections	0.3%	0.3%	<ul> <li>Collect more data with reflections</li> <li>Add synthetic reflections to train set</li> <li>Try to remove with pre-processing</li> <li>Better sensors</li> </ul>	Medium
3. Nighttime scenes	0.1%	1%	<ul> <li>Collect more data at night</li> <li>Synthetically darken training images</li> <li>Simulate night-time data</li> <li>Use domain adaptation</li> </ul>	High

## Domain adaptation

#### What is it?

Techniques to train on "source" distribution and generalize to another "target" using only unlabeled data or limited labeled data

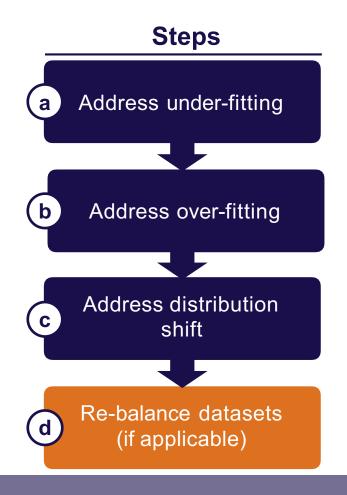
#### When should you consider using it?

- Access to labeled data from test distribution is limited
- Access to relatively similar data is plentiful

# Types of domain adaptation

Туре	Use case	Example techniques
Supervised	You have limited data from target domain	<ul><li>Fine-tuning a pre- trained model</li><li>Adding target data to train set</li></ul>
Un-supervised	You have lots of unlabeled data from target domain	<ul><li>Correlation Alignment (CORAL)</li><li>Domain confusion</li><li>CycleGAN</li></ul>

## Prioritizing improvements (i.e., applied b-v)

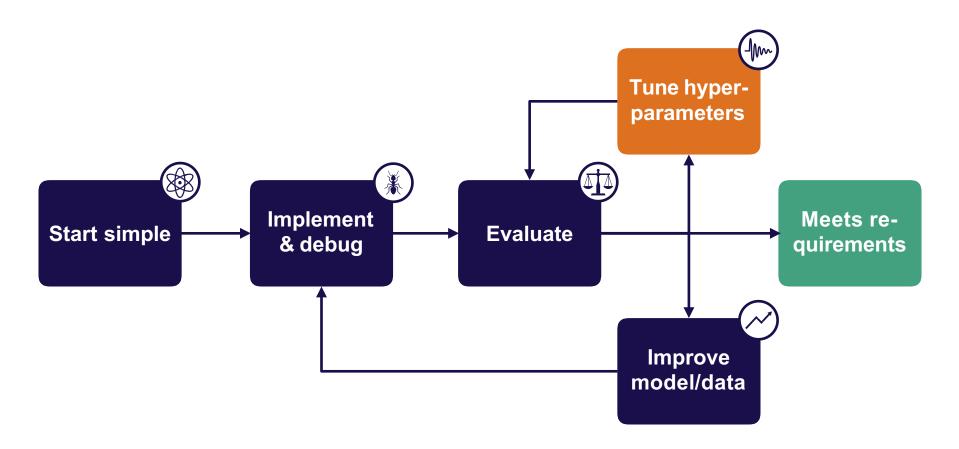


# Rebalancing datasets

- If (test)-val looks significantly better than test, you overfit to the val set
- This happens with small val sets or lots of hyper parameter tuning
- When it does, recollect val data

Questions?

# Strategy for DL troubleshooting



**I**m Troubleshooting - tune

# Hyperparameter optimization

#### Model & optimizer choices?

#### **Network:** ResNet

- How many layers?
- Weight initialization?
- Kernel size?
- Etc

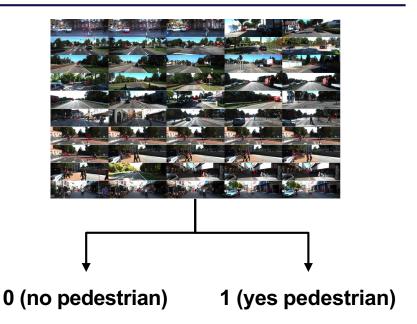
#### **Optimizer:** Adam

- Batch size?
- Learning rate?
- beta1, beta2, epsilon?

#### Regularization

- . . . .

#### Running example



Goal: 99% classification accuracy

# Which hyper-parameters to tune?

#### **Choosing hyper-parameters**

- More sensitive to some than others
- Depends on choice of model
- Rules of thumb (only) to the right
- Sensitivity is relative to default values!
   (e.g., if you are using all-zeros weight initialization or vanilla SGD, changing to the defaults will make a big difference)

Approximate sensitivity
High
High
Low
Low
Low
Medium
High
Medium
High
Medium
Medium
Low

## Method 1: manual hyperparam optimization

#### How it works

- Understand the algorithm
  - E.g., higher learning rate means faster less stable training
- Train & evaluate model
- Guess a better hyperparam value & reevaluate
- Can be combined with other methods (e.g., manually select parameter ranges to optimizer over)

#### **Advantages**

 For a skilled practitioner, may require least computation to get good result

#### **Disadvantages**

- Requires detailed understanding of the algorithm
- Time-consuming

# Method 2: grid search

#### How it works

#### **Advantages**

- Super simple to implement
- Can produce good results

#### **Disadvantages**

- Not very efficient: need to train on all cross-combos of hyperparameters
- May require prior knowledge about parameters to get good results

Hyperparameter 2 (e.g., learning rate)

Hyperparameter 1 (e.g., batch size)

# Method 3: random search

### **How it works**

Hyperparameter 2 (e.g., learning rate)

### **Advantages**

- Easy to implement
- Often produces better results than grid search

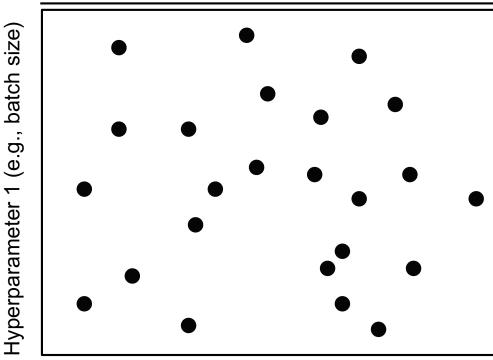
### **Disadvantages**

- Not very interpretable
- May require prior knowledge about parameters to get good results

Hyperparameter 1 (e.g., batch size)

### **How it works**

## \_\_\_\_\_ Advantages

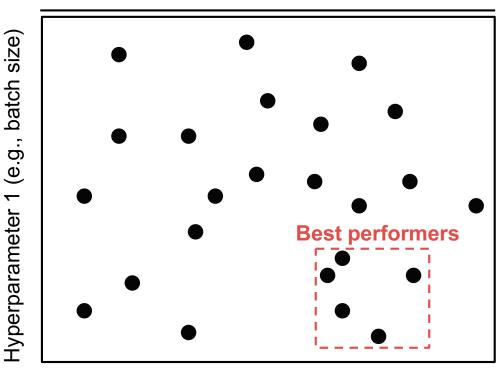


**Disadvantages** 

Hyperparameter 2 (e.g., learning rate)

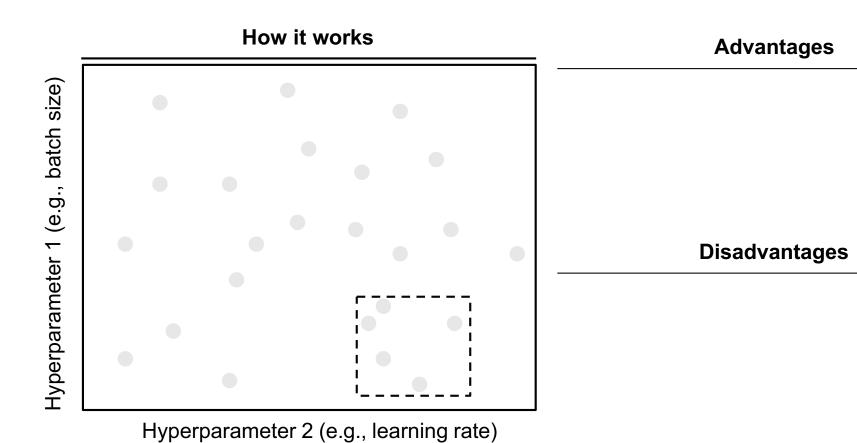
### How it works

### **Advantages**



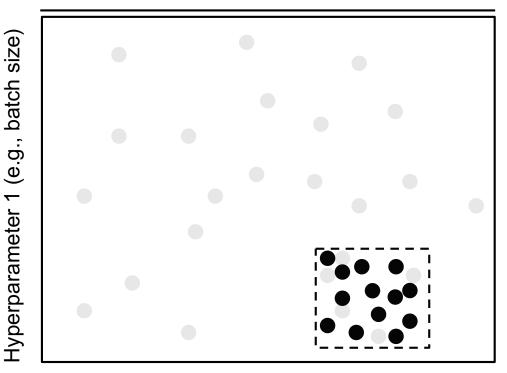
**Disadvantages** 

Hyperparameter 2 (e.g., learning rate)



# How it works

### **Advantages**



**Disadvantages** 

Hyperparameter 2 (e.g., learning rate)

### How it works

# etc.

### **Advantages**

- Can narrow in on very high performing hyperparameters
- Most used method in practice

### **Disadvantages**

Somewhat manual process

Hyperparameter 1 (e.g., batch size)

# Method 5: Bayesian hyperparam opt

### How it works (at a high level)

- Start with a prior estimate of parameter distributions
- Maintain a probabilistic model of the relationship between hyper-parameter values and model performance
- Alternate between:
  - Training with the hyper-parameter values that maximize the expected improvement
  - Using training results to update our probabilistic model
- To learn more, see:

### **Advantages**

 Generally the most efficient hands-off way to choose hyperparameters

### **Disadvantages**

- Difficult to implement from scratch
- Can be hard to integrate with off-the-shelf tools

https://towards datascience.com/a-conceptual-explanation-of-bayesian-model-based-hyperparameter-optimization-for-machine-learning-b8172278050 for the conceptual-explanation of the conc

# Method 5: Bayesian hyperparam opt

### How it works (at a high level)

- Start with a prior estimate of parameter distributions
- Maintain a probabilistic model of the relationship between hyper-parameter values and model p
- Alternate between:
  - values that maxir improvement

 Using training results to update our probabilistic model

### **Advantages**

 Generally the most efficient hands-off way to choose hyperparameters

More on tools to do this automatically inadvantages Training with the hypernearameter ucture & tooling lecture!

ent from scratch

<del>can be nare to int</del>egrate with off-the-shelf

tools

To learn more, see:

https://towardsdatascience.com/a-conceptual-explanation-of-bayesian-model-based-hyperparameter-optimization-for-machine-learning-b8172278050f

# Summary of how to optimize hyperparams

- Coarse-to-fine random searches
- Consider Bayesian hyper-parameter optimization solutions as your codebase matures

Questions?

# Conclusion

- DL debugging is hard due to many competing sources of error
- To train bug-free DL models, we treat building our model as an iterative process
- The following steps can make the process easier and catch errors as early as possible

Troubleshooting - conclusion 15

# How to build bug-free DL models



• Choose the simplest model & data possible (e.g., LeNet on a subset of your data)



Once model runs, overfit a single batch & reproduce a known result



 Apply the bias-variance decomposition to decide what to do next



Use coarse-to-fine random searches



 Make your model bigger if you underfit; add data or regularize if you overfit

**Troubleshooting - conclusion** 

