Design patterns for Machine Learning

Exploration report by Szymon Jessa

2017-10-23, mlgdansk

Best practices? Design patterns for Machine Learning

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2017-10-23, mlgdansk

Reference

Explored:

- Leslie N. Smith, Best Practices for Applying Deep Learning to Novel Applications, https://arxiv.org/abs/1704.01568
- Andrew Ng, *Structuring Machine Learning Projects*, https://www.coursera.org/learn/machine-learning-projects/home/welcome
- Andrew Ng, *Machine Learning*, https://www.coursera.org/learn/machine-learning
- Martin Zinkevich, Rules of Machine Learning: Best Practices for ML Engineering,
 http://martin.zinkevich.org/rules_of_ml/rules_of_ml.pdf
- Robert Chu, David Duling, Wayne Thompson, *Best Practices for Managing Predictive Models in a Production Environment*, http://www2.sas.com/proceedings/forum2007/076-2007.pdf

Not yet explored:

- More than 10 other papers/pages/lessons
- DO YOU HAVE ANY RECOMMENDATIONS?

Design patterns? But I know everything already...

ML Superhero: My great model achieved 90% accuracy.

CEO: Nice, but we need 95%. What can we do?

ML Superhero: I have plenty of ideas what we could do:

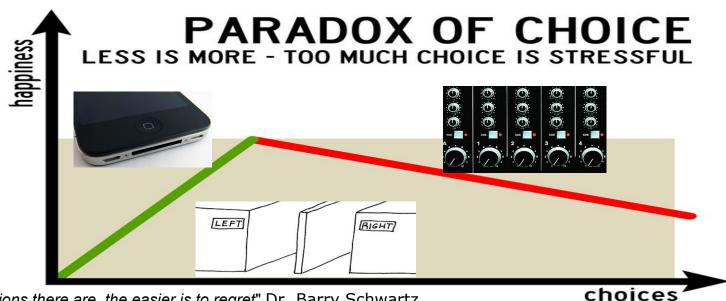
- so we can address the bias
- try a **bigger network**
- or maybe we **overfit**
- we could ask Martin for more data
- or do data augmentation
- use **regularization**
- maybe **dropout**
- check the alternative **features extraction**
- review some recent papers from competition
- try the **novel idea** I have...

CEO: Nice, but we have **no time** to check everything, so which of these makes **most sense** to do now? **ML Superhero:** Ok... Let me check in the "*Design patterns for Machine Learning*" presentation...

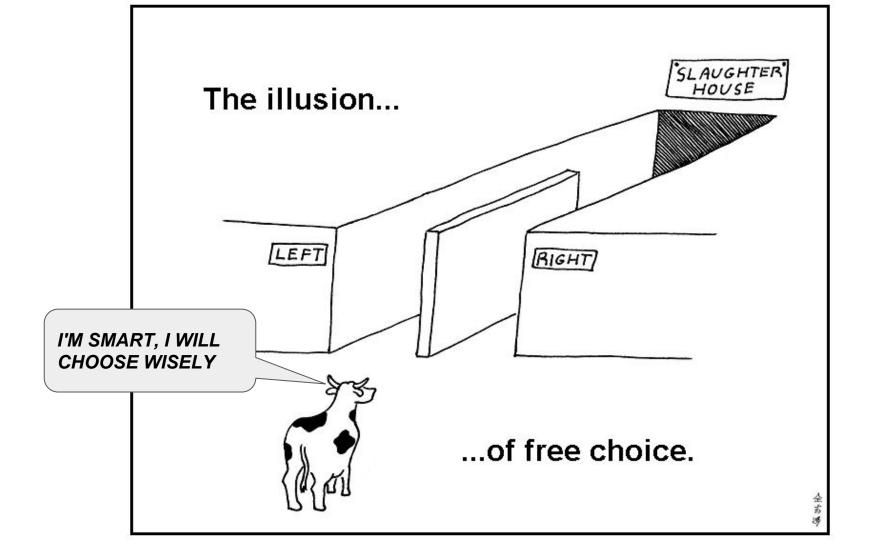
Root cause? I'm just too smart...?

TOO -SO many options

Single variable/parameter affects multiple things



"The more options there are, the easier is to regret" Dr. Barry Schwartz https://www.ted.com/talks/barry_schwartz_on_the_paradox_of_choice/transcript



Orthogonalization

MAKE SINGLE KNOB RESPONSIBLE FOR CHANGING SINGLE THING MAKE IT EASY TO UNDERSTAND





ML EXPERTS KNOW WHICH KNOB TO USE TO MAKE THE DESIRED CHANGE

Orthogonalization on high level



Define the metric for what you aim to achieve



Build a model that will fit the target

Build your first system quickly, then iterate.

Build **solid** end to end **pipeline** (complete system)

Start with **reasonable objective**Add **common sense features** in a simple way

Ensure the **pipeline stays solid**

If machine learning is not **absolutely required** for your product, don't use it until you have data.

If you think that machine learning will give you a 100% boost, then a heuristic will get you 50% of the way there.

But...

If you think that machine learning will give you a 100% boost, then a heuristic will get you 50% of the way there.

But...

Choose machine learning over a complex heuristic:

A complex heuristic is **unmaintainable** - -learned model is easier to update and maintain. Once you have data and a basic idea of the goal, move on to machine learning.

Use bias, variance and error analysis to prioritize next steps.

If there are already solutions for your problem - use them, but don't make it more complex than necessary!

Building an application: Steps

- Step 1. Define goal and set evaluation metric
- Step 2. Prepare data
- Step 3. Baseline model
- Step 4. Environment visualization, debugging
- Step 5. Fine tune model
- Step 6. Increase complexity

Define goal and set evaluation metric

- Define what success look like (either if done by human or computer)
- What is human performance and how the state-of-the art compares to it?
- Make the network's task as easy as possible:
 eg. face detection, face recognition but not face detection + face recognition
 (the easier the job the networks must perform, the easier it will be to train and the better the performance)
- Remember: The scarcest resource is human time so let the network learn its representations rather than require any fixed, manual preprocessing

WHICH MODEL IS BETTER? DID WE IMPROVED WITH MODEL B OR NOT?

Model	Precision	Recall
Α	91%	87%
В	94%	80%

$$ext{Precision} = rac{tp}{tp+fp}$$

$$ext{Recall} = rac{tp}{tp+fn}$$

When ONE is MORE than TWO

Model	Precision	Recall	F-measure
A	91%	87%	89%
В	94%	80%	86%

$$F = 2 \cdot rac{ ext{precision} \cdot ext{recall}}{ ext{precision} + ext{recall}}$$

When ONE is MORE than TWO

Model	Precision	Recall	Fixeasure
A	DITT	87%	89%
ONE	94%	80%	86%

$$F = 2 \cdot rac{ ext{precision} \cdot ext{recall}}{ ext{precision} + ext{recall}}$$

Don't overthink which objective to choose to optimize.

Early in the machine learning process, you will notice all the metrics going up, even those that you do not directly optimize.

Keep it simple until you can still easily increase all the metrics.

Note: Often you don't know the true objective. The ML objective should be something that is easy to measure and is a proxy for the "true" objective.

Human-level performance: coz we are the best...

Why it is good to know the human-level performance?

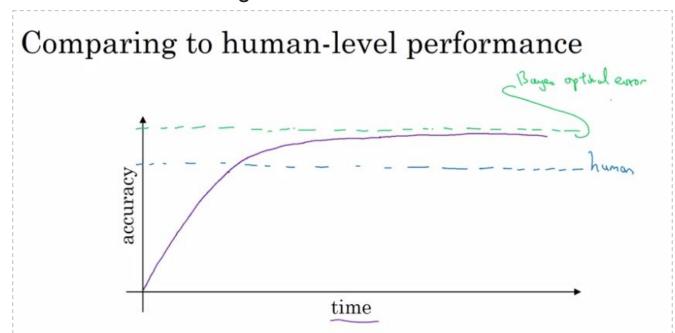
If the model performs below or at human-level, you can:

- get manually labeled data
- gain insight from manual error analysis (why did a person get this right?)
- analyse the bias/variance better
- use human-level error as a proxy for Bayes error

Knowing human-level performance, you know how well but not too well you want your algorithm to do on the training set.

Human-level performance vs Bayes error rate

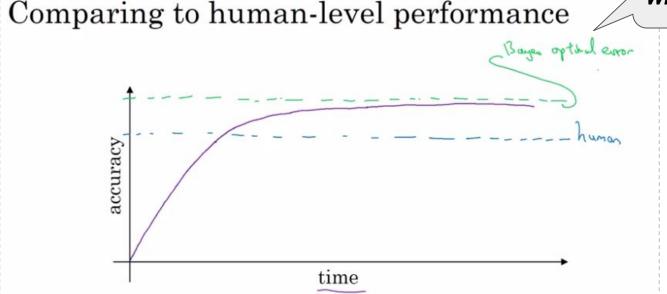
Bayes error rate is the lowest possible error rate for any classifier of a random outcome and is analogous to the irreducible error



Human-level performance vs Bayes error rate

Bayes error rate is the lowest possible error rate for any classifier of a random

outcome and is analogous to the irreducible error



CAN YOU RECOGNIZE WHO WROTE THAT?

Human-level performance: which one?

QUESTION: WHAT IS THE HUMAN-LEVEL ERROR IN THIS EXAMPLE?

QUESTION: WHAT IS THE BAYES ERROR?

Step 2. Prepare data

Make the data wait for YOU - and not the opposite

Before formalizing what your machine learning system will do, track as much as possible in your current system, eg. gain permission from the system's users earlier. If you think that something might be a concern in the future, it is better to get historical data now.

Ensure you are ALLOWED to use the data

Identify legal issues: certain variables might be good predictors, they may result in unwanted risk exposure for an organization when used in a predictive model. For example, there can be legal reasons why variables such as age, gender, and/or race might not be used in the model-building process.

Step 2. Prepare data

Data completeness

- Ensure the data is relevant to the goal
- Ensure that it is diverse enough that it covers the whole problem space
- Check if the classes are balanced

Make the data easy to learn

- Zero mean / normalize the data (removes the need of learning the mean)
- Use a priori knowledge or known heuristics to lower the dimensionality of the data

Step 2. Prepare data

Not enough data?

- Consider transfer learning
- Download datasets that are closest to your data to use for pre-training
- Consider creating synthetic data

Split the data: set up training, dev and test sets

General workflow / data sets use:

- Try a lot of ideas, train different models on the training set,
- and then use the dev set to evaluate the different ideas and pick the best one.
- And you keep innovating to improve **dev set** performance until, finally, you have one model that you're happy with (according to the **evaluation metric**),
- that you then evaluate on your **test set**.

Split the data: size of train, dev and test sets

YOU ALL KNOW THIS ALREADY, RIGHT?

TRAINING SET	DEV SET	TEST SET
60%	20%	20%

and without the test set:

TRAINING SET	DEV SET
80%	20%
70%	30%

Split the data: size of train, dev and test sets

YOU ALL KNOW THIS ALREAD GHT?

TRAINING SET	DEV SET	TEST SET
60%	200	20%

and with the test set:

TRAIN SET	DEV SET
%	20%
70%	30%

Split the data: size of train, dev and test sets

IT IS OK FOR ~100-10k EXAMPLES, BUT WHAT ABOUT 1MLN EXAMPLES?

MAKE THE DEV/TEST BIG ENOUGH TO VERIFY THE OVERALL PERFORMANCE BUT NOT BIGGER

TOTAL NUMBER OF EXAMPLES	TRA	INING SET	D	EV SET	TES	ST SET
10 000	60%	6 000	20%	2 000	20%	2 000
1 000 000	98%	980 000	1%	10 000	1%	10 000

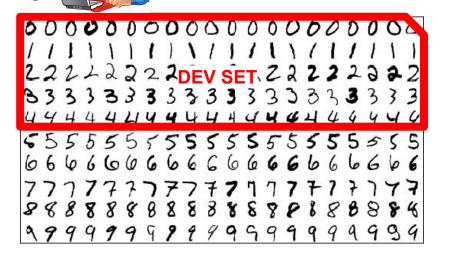
HAVING 1M EXAMPLES, WITH 1% WE STILL GET ENOUGH! ...

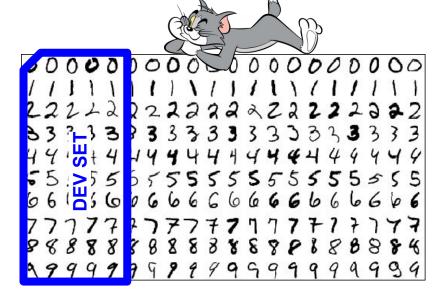
... AND WE WILL ENJOY THE TRAINING DATA IN DEEP LEARNING

Split the data: in dev/test sets balance is the key

IMAGINE: BOTH YOU AND TOM ACHIEVED 100% ACCURACY ON YOUR DEV SETS.

AND GUESS WHO WILL GET MORE CUSTOMER COMPLAINS?



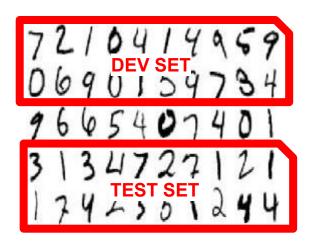


Split the data: in dev/test sets balance is the key

GUIDELINE: ENSURE DEV AND TEST SETS REFLECT THE DATA (INC. DISTRIBUTION)

EXPECTED IN THE TARGET ENVIRONMENT

BEST PRACTICE: SHUFFLE THE DATA AND SPLIT IT THEN INTO DEV AND TEST SET



What to do with incorrectly labelled examples in training data set?

Deep learning algorithms are robust to random errors

(**SOME** white dogs labelled as cat),

but are **prone to systematic errors**

(**ALL** white dogs labelled as cat).

What to do with incorrectly labelled examples in **dev or test set**? When do we need to fix them?

Do error analysis:

- get 100 incorrectly classified examples
- count how many of the incorrect classifications are due to an incorrect label
- calculate how much they affect the dev set error (eg. 6 wrong labels in 100 errors = 6%; 6% of 10% => 0.6%)

	PROJECT ALPHA	PROJECT BETA
DEV SET ERROR	10%	2%
ERRORS DUE TO INCORRECT LABELS	0.6%	0.6%
IS IT WORTH FIXING LABELS?	? Do you know?	

What to do with incorrectly labelled examples in **dev or test set**? When do we need to fix them?

GUIDELINE: Fix labels, only if it makes significant difference

	PROJECT ALPHA	PROJECT BETA
DEV SET ERROR	10%	2%
ERRORS DUE TO INCORRECT LABELS	0.6% => 9.4%	0.6% => 1.4%
IS IT WORTH FIXING LABELS?	MAYBE NOT YET?	YES!

What to do with incorrectly labelled examples in **dev or test set**? When do we need to fix them?

GUIDELINE: Fix labels, only if it males THEM AT ALL? difference BUT WAIT! WHY DO WE NEED TO FIX THEM AT ALL? difference

	PROJECT ALPHA	PROJECT BETA
DEV SET ERROR	10%	2%
ERRORS DUE TO INCORRECT LABELS	0.6% => 9.4%	0.6% => 1.4%
IS IT WORTH FIXING LABELS?	MAYBE NOT YET?	YES!

Cleaning data: concerns with incorrect labels

BUT WAIT! WHY DO WE NEED TO FIX THEM AT ALL?

	MODEL ALPHA	MODEL BETA
DEV SET ERROR	10%	5%
	CAN YOU TELL WHI	CH ONE IS BETTER?

Cleaning data: concerns with incorrect labels

BUT WAIT! WHY DO WE NEED TO FIX THEM AT ALL?

	MODEL ALPHA	MODEL BETA
DEV SET ERROR	10%	5%
ERRORS DUE TO INCORRECT LABELS	80% => 80% * 10% = 8%	20% => 20% * 5% = 1%
	CAN YOU TELL WHI	CH ONE IS BETTER? 38

Cleaning data: concerns with incorrect labels

RECALL: The **dev set** is used to compare models (MODEL ALPHA or MODEL BETA?).

If due to incorrectly labelled examples the error is too high, the **dev set** error won't be a valid way to compare models.

BUT WAIT! WHY DO WE NEED TO FIX THEM AT ALL?

	MODEL ALPHA	MODEL BETA
DEV SET ERROR	10%	5%
ERRORS DUE TO INCORRECT LABELS	80% => 8% (best: 2%)	20% => 1% (best: 4%)
	CAN YOU TELL WHICH ONE IS BETTER?	

Create a simple baseline model

- Keep the first model simple: The first model provides the biggest boost to your product, so it doesn't need to be fancy.
- Some teams aim for a "neutral" first launch: a first launch that explicitly deprioritizes machine learning gains, to avoid getting distracted.
- Use one framework and one computer language to minimize complexity
- Find similar application or paper and replicate the results
- Use a smaller architecture than you anticipate you might need
- Use only part of the training data
- Get only the **basic functionality** now
- Adopt some of the practices of agile software methodologies

Use simple features

Start with directly observed and reported features as opposed to learned features.

AND EVERYONE KNOWS WHAT A "LEARNED FEATURE" IS...

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AND EVERYONE KNOWS WHAT A "LEARNED FEATURE" IS...

A learned feature is a feature generated either by an external system (such as an unsupervised clustering system) or by the learner itself (e.g. via deep learning).

Use simple features

Start with directly observed and reported features as opposed to learned features.

AND EVERYONE KNOWS WHAT A "LEARNED FEATURE" IS...

A learned feature is a feature generated either by an external system (such as an unsupervised clustering system) or by the learner itself (e.g. via deep learning).

Turn heuristics into features

transition to a machine learned system will be smoother usually those rules contain a lot of the intuition about the system

... BUT HOW?

Turn heuristics into features

Preprocess using the heuristic

spam filter: if the sender has already been blacklisted, don't try to relearn what "blacklisted" means

Create a feature directly from the heuristic

use a heuristic to compute a relevance score for a query result as the value of a feature

Decompose a complex heuristic

If there is a heuristic for apps that combines the number of installs, the number of characters in the text, and the day of the week, then consider pulling these pieces apart, and feeding these inputs into the learning separately.

But... Using old heuristics in new machine learning algorithm can help to create a smooth transition, but think about whether there is a simpler way to accomplish the same effect.

Choose the algorithm with respect to your business needs

The trade-off between interpretability and prediction accuracy must be carefully considered at this stage.

Certain models such as decision trees produce results that are easy to be interpreted. They enable you to answer questions like "Why was this customer denied credit?" Other models such as neural networks do not provide this sort of simple interpretation and hence might be inappropriate for certain applications.

Step 4. Environment - visualization, debugging

- Your level of understanding what is happening in the model will affect the success of your project
- Visualize your architecture and measure internal entities to understand why you are getting the results you are obtaining
- Set up visualizations so you can monitor as much as possible while the architecture evolves
- Create unit tests for all of your code modifications

Step 4. Environment - visualization, debugging

Test the infrastructure independently from the machine learning

Make sure that the infrastructure is testable, and that the learning parts of the system are encapsulated so that you can test everything around it. Machine learning has an element of unpredictability, so make sure that you have tests for the code for creating examples in training and serving, and that you can load and use a fixed model during serving

Audit validation processes: Every step of the validation process needs to be logged

For example: who imported what model when; who selected what model as the champion model, when and why; who reviewed the champion model for compliance purposes; and who published the champion to where and when.

Monitor the model

A champion predictive model is deployed for a period of time in production environments. A champion model needs to retire when its performance degradation hits a certain threshold. Typically, model performance degrades over time.

Track input and output variable distribution shifts

Step 4. Environment - visualization, debugging

Watch for silent failures

Suppose that a particular table that is being joined is no longer being updated. The machine learning system will adjust, and behavior will continue to be reasonably good, decaying gradually. Sometimes tables are found that were months out of date, and a simple refresh improved performance. For example, the coverage of a feature may change due to implementation changes: for example a feature column could be populated in 90% of the examples, and suddenly drop to 60% of the examples. Play once had a table that was stale for 6 months, and refreshing the table alone gave a boost of 2% in install rate. If you track statistics of the data, as well as manually inspect the data on occassion, you can reduce these kinds of failures.

Give feature column owners and documentation

If the system is large, and there are many feature columns, know who created or is maintaining each feature column.

- This will take the most time you will experiment extensively
- Apart from factors you believe will improve the result try changing every factor to learn what happens when it changes
- The objectives you defined in step 1 should guide how far you want to pursue the performance improvements.
- During this phase, all of the metrics should still be rising.
- Or you may revise the objectives your defined earlier.

Use existing features to create new features in human- understandable ways Discretization

Taking a continuous feature and creating many discrete features from it.

Example: Consider a continuous feature such as age. You can create a feature which is 1 when age is less than 18, another feature which is 1 when age is between 18 and 35 etc. Don't overthink the boundaries of these histograms: basic quantiles will give you most of the impact.

Cross combination of two or more feature columns

A feature column, in TensorFlow's terminology, is a set of homogenous features, (e.g. {male, female}, {US, Canada, Mexico}, etc.). A cross is a new feature column with features in, for example, {male, female} × {US,Canada, Mexico}. This new feature column will contain the feature (male, Canada).

Note that it takes massive amounts of data to learn models with crosses of three, four, or more base feature columns. Crosses that produce very large feature columns may overfit.

Use very specific features when you can

With tons of data, it is simpler to learn millions of simple features than a few complex features. Don't be afraid of groups of features where each feature applies to a very small fraction of your data, but overall coverage is above 90%. You can use regularization to eliminate the features that apply to too few examples.

Avoid feedback loops with positional features

The position of content dramatically affects how likely the user is to interact with it. If you put an app in the first position it will be clicked more often, and you will be convinced it is more likely to be clicked

Clean up features you are no longer using

Unused features create technical debt. If you find that you are not using a feature, and that combining it with other features is not working, then drop it out of your infrastructure.

Keep coverage in mind when considering what features to add or keep

How many examples are covered by the feature? Some features may punch above their weight. For example, if you have a feature which covers only 1% of the data, but 90% of the examples that have the feature are positive, then it will be a great feature to add.

The number of features you can learn in a linear model is roughly proportional to the amount of data you have

1 000 examples -> a dozen features

10 000 000 examples -> hundred thousand features

billions or hundreds of billions of examples -> 10 million features

Iterate from the first to the last component in the pipeline:

assume that the component gets 100% accuracy -> and evaluate the system.

OCR pipeline: text detection, character segmentation, character recognition.

	Step	System accuracy	Change
Actu	al system performance	72%	
+	Perfect text detection		
+	Perfect character segmentation		
+	Perfect character recognition		

Iterate from the first to the last component in the pipeline:

- assume that the component gets 100% accuracy -> and evaluate the system.

OCR pipeline: **text detection**, character segmentation, character recognition.

Step	System accuracy	Change
Actual system performance	72%	
+ Perfect text detection	89%	+17%
+ Perfect character segmentation		
+ Perfect character recognition		

Iterate from the first to the last component in the pipeline:

assume that the component gets 100% accuracy -> and evaluate the system.

OCR pipeline: text detection, character segmentation, character recognition.

Step	System accuracy	Change
Actual system performance	72%	
+ Perfect text detection	89%	+17%
+ Perfect character segmentation	90%	+1%
+ Perfect character recognition		

Iterate from the first to the last component in the pipeline:

- assume that the component gets 100% accuracy -> and evaluate the system.

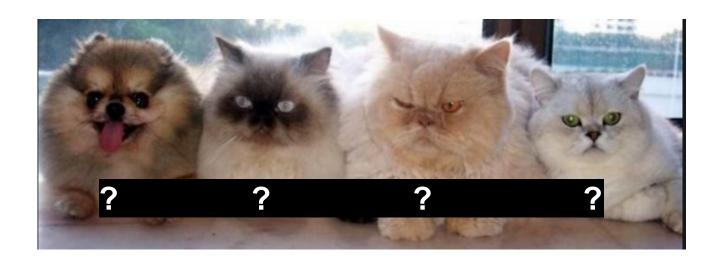
Look for the biggest change in accuracy.

	Step	System accuracy	Change
Actu	al system performance	72%	
+	Perfect text detection	89%	+17%
+	Perfect character segmentation	90%	+1%
+	Perfect character recognition	100%	+10%

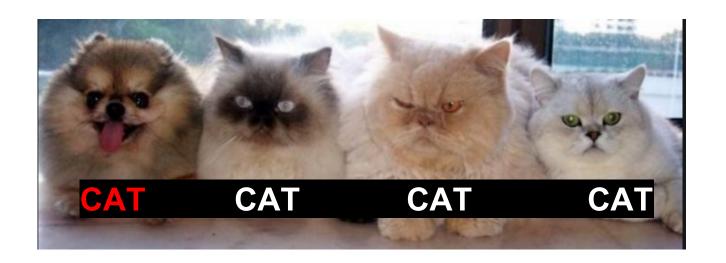
It shows which component significantly impacts the performance (text detection). And which component - even if 100% accurate - won't help much (segmentation).

Step	System accuracy	Change
Actual system performance	72%	
+ Perfect text detection	89%	+17%
+ Perfect character segmentation	90%	+1%
+ Perfect character recognition	100%	+10%

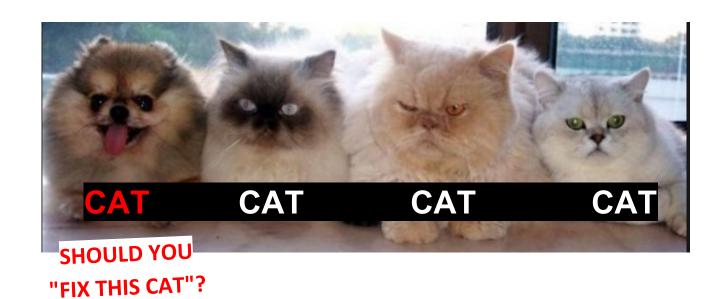
Detect cats



Detect cats



Detect cats



61

Get insight examining mistakes **manually**.

- 1. Get ~100 misrecognized dev set examples
- 2. Count how many cats are actual dogs
- 3. Evaluate the impact on the performance

EXAMPLE		
Error rate	10%	
Number of dogs in the 100 misrecognized dev set examples	5 (5 in 100 = 5%)	
Estimated error rate in best case after improvement	9.5% (5% of 10% = 0.5%)	



Try to quantify observed undesirable behavior

The general rule is "measure first, optimize second"

Don't fix just because someone in your team says it is important. Let the numbers speak.

Look for patterns in the measured errors and create new features

If you give the model a feature that allows it to fix the error, the model will try to use it.

If you try to create a feature based upon examples the system doesn't see as mistakes, the feature will be ignored.

If you are going to add post length, don't try to guess what long means - let the model figure it out.

You are not a typical end user - While a change which is obviously bad should not be used, anything that looks reasonably near production should be tested further, either by paying laypeople to answer questions on a crowdsourcing platform, or through a live experiment on real users. There are two reasons for this:

- you are too close to the code. You may be looking for a particular aspect of the posts, or you are simply too emotionally involved (confirmation bias)
- o your time is too valuable. Consider the cost of 9 engineers sitting in a one hour meeting, and think of how many contracted human labels that buys on a crowdsourcing platform

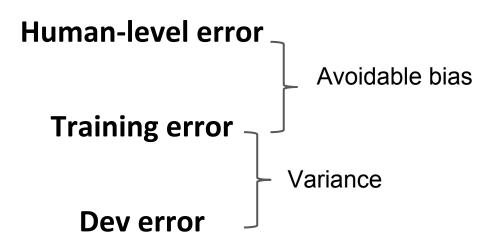
- Be aware that identical short-term behavior does not imply identical long-term behavior.

Human-level performance: coz we are the best...

Human-level performance tells you how well your algorithm may fit the training set

(and we know that is achievable - because humans can do it)

Human-level error serves as an approximation for Bayes error rate (the minimal error)



Reduce bias or variance: what to do next?

	Project Alpha	Project Beta
Training set error	8%	8%
Dev set error	10%	10%





Reduce bias or variance: what to do next?

	Project Alpha	Project Beta
Training set error	8%	8%
Dev set error	10%	10%
Human-level error	1%	7,5%

Two fundamental assumptions of supervised learning:

You can fit the training set pretty well (via working on reducing avoidable bias)
The training set performance generalizes pretty well to the dev/test set (via working on reducing variance)

Reduce bias or variance: what to do next?

	Project Alpha	Project Beta
Training set error	8%	8%
Dev set error	10%	10%
Human-level error	1%	7,5%

Try reducing **bias** (training set error)

Try reducing **variance** (dev set error, generalization)

Reduce bias or variance: but how?

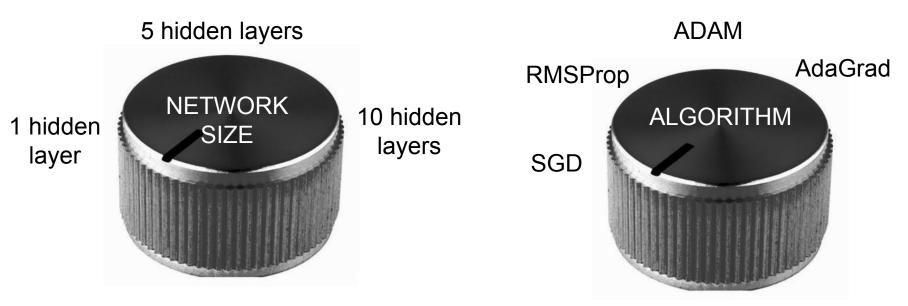
To reduce avoidable bias (human-level error vs training set error)

- Train bigger/higher dimensional model
- Use another optimization algorithm (Momentum, RMSProp, Adam etc.)
- Try another NN architecture/change hyperparameters (RNN, CNN, LSTM etc.)

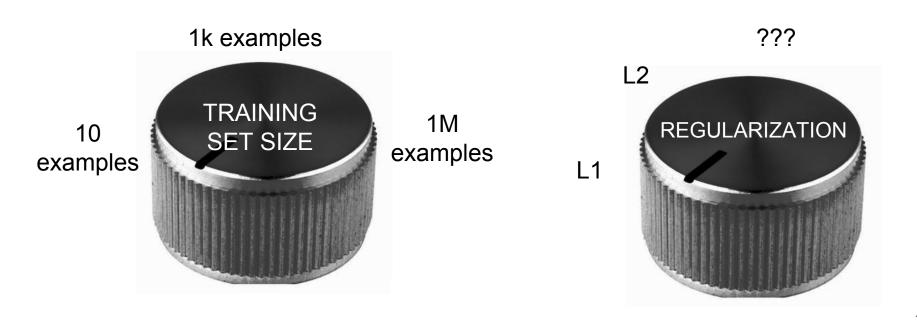
To reduce variance (training error vs dev set error)

- Get more data (to generalize better)
- Use regularization (L2, dropout, data augmentation add noise)
- Try another NN architecture/change hyperparameters

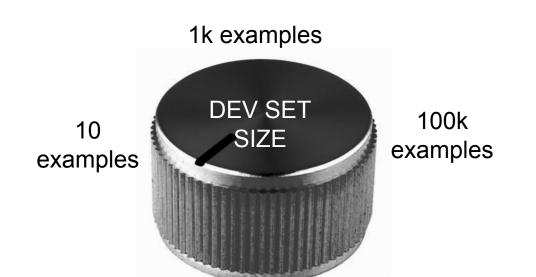
To fit training set well (eg. achieve human-level performance)



Fit dev set (model fits the training set well but fails to generalize)



Fit test set (model fits train and dev sets, but fails on test set)



you probably overfit on the dev set, try to add more examples to it

Your model fits the training, dev and test set, but doesn't perform well in real world



Does the data (distribution) reflect the real world distribution?



Does the metric correctly reflect the real goal?

Step 6. Increase complexity

If you have the time and budget, you can investigate more complex methods and there are worlds of complexities that are possible.

Two common methods to consider:

end-to-end training and ensembles

Step 6. Increase complexity

DO YOU HAVE IT?

If you have the time and budget, you can investigate more complex methods and there are worlds of complexities that are possible.

Two common methods to consider:

end-to-end training and ensembles

Step 6. Increase complexity

SORRY, NO TIME

WORK IN PROGRESS!

COME BACK LATER:)

Conclusion?

THEY DAY IS TOO SHORT