Lecture 12
Mechanisms of Training and Running Neural Nets
Announcements

• Pset 4 due today
• Pset 5 out today
12. Mechanisms of Training and Running Neural Nets

- Data
- Model
- Optimization
- Evaluation, Execution, and Debugging

Lots of slides adapted from Evan Shelhamer’s “DIY Deep Learning: Advice on Weaving Nets”
Data

Machine learning == Data-driven intelligence
“Become friends with every pixel”
“Become friends with every pixel”

Look at your data
Look at the output

Look at the filters

Visualize neurons

Loss

epoch
Data

Look at the data!

inspect the distribution of inputs and targets

• inspect random selection of inputs and targets to have a general sense

• histogram input dimensions to see range and variability

• histogram targets to see range and imbalance

• select, sort, and inspect by type of target or whatever else

[slide adapted from Evan Shelhamer]
Data

Inspect the inliers, outliers, and neighbors:

• visualize distribution and data, especially **outliers**, to uncover dataset issues

• look at **nearest neighbors**

• examples:
  
  • rare grayscale images in color dataset, huge images that should have been rescaled, corrupted class labels that had been cast to uint8

[slide adapted from Evan Shelhamer]
Data

pre-processing: the data as it is loaded is not always the data as it is stored!

• inspect the data as it is given to the model by \( \text{output} = \text{model}\text{(data)} \)

[slide adapted from Evan Shelhamer]
Data

pre-processing:

• **standardize:**

\[
x_k \leftarrow \frac{x_k - \mathbb{E}[x_k]}{\sqrt{\text{Var}[x_k]}} \quad \forall k
\]

• Squashes all your data dimensions into the same standard range

• This makes it so that, a priori, no one dimension is valued more than any other

• Important when different measurements have vastly different scales or units
Data

pre-processing:

• **summary statistics**: check the min/max and mean/variance to catch mistakes like loading values in the range $[0,255]$ when the model expects values in the range $[0,1]$.

• **shape**: are you certain of each dimension and its size?
  
  • sanity check with dummy data of prime dimensions: there are no common factors, so mistaken reshaping/flattening/permuting will be more obvious. example: a 64x64x64x64 array can be permuted without knowing

• **type**: check for casting, especially to lower precision
  
  • what's -1 for a byte? how does standardization change integer data?
Data

resample the data to decorrelate: that is, remember to **shuffle**

- when you shuffle your inputs, $x$, make sure your targets, $y$, are shuffled in the same order!

consider selecting miniature train and test sets for development and testing: these should be chosen once and fixed throughout optimization + evaluation

- it's heartbreaking to wait an entire epoch and then and only then have your experiment-to-be crash

[slide adapted from Evan Shelhamer]
Data

check if you can do the task, as it is given to the model

• take windowed data at receptive field size

... see if it's a reasonable perceptual task for a human

[slide adapted from Evan Shelhamer]
Data augmentation

Training data:

- $x$, “Fish”
- $x$, “Grizzly”
- $x$, “Chameleon”
- ...

- $y$, “Fish”
- $y$, “Fish”
- $y$, “Fish”

Transformations:
- Mirror
- Crop
- Crop
- Darken
Idea: Train on randomly perturbed data, so that test set just looks like another random perturbation.

This is called **domain randomization** or **data augmentation**.
Domain randomization

Training data

Test data

[Sadeghi & Levine 2016]
Above example is from [Tobin et al. 2017]
Domain gap between $p_{source}$ and $p_{target}$ will cause us to fail to generalize.
OpenAI Dactyl

[https://openai.com/blog/learning-dexterity/]
OpenAI Dactyl

FINGER PIVOTING

SLIDING

FINGER GAITING

[https://openai.com/blog/learning-dexterity/]
Model

Keep it as simple as possible!

sure, there are sophisticated models out there

but they were made by either

1) going step-by-step, from simple to complex, or

2) suffering, madness, and the gnashing of teeth

[slide adapted from Evan Shelhamer]
Model

Keep it as simple as possible!

Why keep it simple?

- easy to build, debug, share
- tractable to understand, make robust, build theories around
- *simple models also work better* (Occam’s razor, Solomonoff Induction)
- My personal opinion: simplicity is highly undervalued in the community; if you focus on simplicity you will have an unfair advantage
Model

do your first experiment with the simplest possible model w/ and w/o your idea

if you have a classification problem, you might try:

```python
model = torch.hub.load('pytorch/vision:v0.9.0', 'resnet18')
```

if you have a detection problem, you might try:

```
git clone https://github.com/roytseng-tw/mask-rcnn.pytorch.git
```

find popular models and code here: https://paperswithcode.com/

[slide adapted from Evan Shelhamer]
**Model**

*double-check the model* actually is what you thought you defined

```python
# walk the model for inspection
for name_, module_ in model.named_modules():
    if name_ == 'name' or isinstance(module_, nn.Conv2d):
        [...]
```

[slide adapted from Evan Shelhamer]
Model

simple baselines catch many issues and swiftly too

• learn a linear model on random features by freezing all the parameters at their initialization except for the final output layer

• zero out the data by \texttt{x.zero()} and check that the results are worse

[slide adapted from Evan Shelhamer]
Model

Transform your problem into a “solved” problem

- Case study: transforming image colorization to image classification

[c.f. the strategy of “polynomial-time reduction”]
Image colorization

\[
\text{Input } \mathbf{x} \quad \rightarrow \quad \text{Output } \mathbf{y}
\]

\[
\arg \min_{f \in \mathcal{F}} \sum_{i=1}^{N} \mathcal{L}(f(\mathbf{x}^{(i)}, \mathbf{y}^{(i)}))
\]

[Zhang, Isola, Efros, ECCV 2016]
Grayscale image: \textbf{L channel}
\[ \mathbf{x} \in \mathbb{R}^{H \times W \times 1} \]

Color information: \textbf{ab channels}
\[ \mathbf{y} \in \mathbb{R}^{H \times W \times 2} \]

[Zhang, Isola, Efros, ECCV 2016]
Grayscale image: **L channel**

\[ x \in \mathbb{R}^{H \times W \times 1} \]

Color information: **ab channels**

\[ y \in \mathbb{R}^{H \times W \times 2} \]

[Zhang, Isola, Efros, ECCV 2016]
Colorization $\rightarrow$ Classification

\[ f \rightarrow \text{yellow} \]
Colors \( \rightarrow \) Classes

\[
y \in \mathbb{R}^{H \times W \times 2}
\]

One hot codes:
- \text{Blue} \rightarrow [0,0,1, \ldots]
- \text{Yellow} \rightarrow [1,0,0, \ldots]
- \text{Pink} \rightarrow [0,1,0, \ldots]

one-hot representation of K discrete classes

\[
y \in \mathbb{R}^{H \times W \times K}
\]
“rockfish”
Image classification $\rightarrow$ Pixel classification

diagram with arrows and a box labeled "yellow"
Image classification $\rightarrow$ Pixel classification

![Diagram showing image classification process]
Image classification $\rightarrow$ Pixel classification
Recipe for deep learning in a new domain

1. Transform your data into numbers (e.g., one-hot vectors)

2. Transform your goal into an numerical measure (e.g., cross-entropy loss)

3. Use a generic optimizer (SGD) and an standard architecture (e.g., CNN) to solve the learning problem
Model

Remember that often the easiest way to get better performance is:

1) **Scale** your data: more (diverse) training examples

2) **Scale** your model: more layers, more channels

3) **Scale** your compute: train for longer

In the current era, I would say these are the top three factors that determine success, roughly in order

… but working at small scale forces efficiency, and *then* when you do scale up, you get more bang for your buck
we are still learning how to optimize deep nets

much progress is being made but it’s nevertheless a dark forest

explore if you like, but balance exploration by exploitation of a known good setting, or the closest setting you can find
Optimization

figure out optimization on one/few/many datapoints, in that order

• overfit to a data point

• then fit a batch

• and finally try fitting the dataset (or a miniature version of it)

first make sure you can fit train set, then consider generalization to test set

[slide adapted from Evan Shelhamer]
Optimization

**sanity check the loss** against a suitable reference value

- classification with cross-entropy loss: uniform distribution

- get to know log loss numbers:
  
  $-0.69 = \ln(0.5)$ [chance on binary classification]

  $-2.3 = \ln(0.1)$ [chance on 10-way classification]

- regression with squared loss: mean of targets (or even just zero)

and if your loss is constant, double check for zero initialization of the weights

[slide adapted from Evan Shelhamer]
Optimization

the **learning rate** and the **batch size** are more-or-less the cardinal hyperparameters

- choose the learning rate on a small set (see Bottou)
- simplify your life and **use a constant rate**, that is, no schedule until everything else is figured out
- schedule according to epochs (== number of passes through the data), not number of iterations of SGD
- set batch size to be as large as will fit in memory

[slide adapted from Evan Shelhamer]
clear gradients after each iteration or else they accumulate (in Pytorch)

remember `opt.zero_grad()`!

remarkably, with adaptive optimizers and enough time a model can still learn if the gradients are never cleared out… but it's really sensitive

[slide adapted from Evan Shelhamer]
checkpoint features + gradients to trade space for time and fit large models

- can then accumulate gradients across checkpoints
- can resume training if your computer crashes
- have a “paper trail” to debug later

[slide adapted from Evan Shelhamer]
Optimization

live on the edge and try extreme settings (but just a little bit)

• If optimization never diverges, your learning rate is too low

in the style of Umeshism

• If you’ve never missed a flight, you’re spending too much time in airports

[slide adapted from Evan Shelhamer]
Evaluation

switch to **evaluation mode** by `model.eval()` (Pytorch)

no, really

and check the mode by `model.training`

[slide adapted from Evan Shelhamer]
Evaluation

**know the output!** metrics and summaries can obscure all kinds of issues

- inspect input/output pairs, across min/max/quartiles of the eval metrics
- keep an eye on the output and loss for a chosen set across iterations to have a sense of the learning dynamics (could be the whole validation set)

[slide adapted from Evan Shelhamer]
**Evaluation**

**separate evaluation** from optimization

- save checkpoints at intervals and evaluate them offline
- there are the perils of nondeterminism, batch norm, etc when mixing training and testing
- plus it only slows down training
Tuning

try the scientific method

• change one thing at a time

not the computer scientific method

• change everything every time

(joke courtesy Dave Patterson)
Tuning

to tune hyperparameters (architectural design choices, optimizer parameters, etc) **random search** is better than grid search

Figure 1: Grid and random search of nine trials for optimizing a function \( f(x,y) = g(x) + h(y) \approx g(x) \) with low effective dimensionality. Above each square \( g(x) \) is shown in green, and left of each square \( h(y) \) is shown in yellow. With grid search, nine trials only test \( g(x) \) in three distinct places. With random search, all nine trials explore distinct values of \( g \). This failure of grid search is the rule rather than the exception in high dimensional hyper-parameter optimization.

[https://www.jmlr.org/papers/volume13/bergstra12a/bergstra12a.pdf]  
[slide adapted from Evan Shelhamer]
Execution

don’t be finger-bound! script the optimization + evaluation of your models

every character you type is a chance to make a mistake

also scripting makes the work reproducible!

[slide adapted from Evan Shelhamer]
log everything! especially arguments

```python
import logging

def setup_logging(logfile):
    FORMAT = '[%(asctime)s.%(msecs)03d] %(message)s'
    DATEFMT = '%Y-%m-%d %H:%M:%S'
    logging.root.handlers = []  # clear logging from elsewhere
    logging.basicConfig(level=logging.INFO, format=FORMAT, datefmt=DATEFMT,
                        handlers=[
                            logging.FileHandler(logfile),
                            logging.StreamHandler(sys.stdout)
                        ])
    logger = logging.getLogger()
    return logger
```

```
args = parser.parse_args()
log = setup_logging('log')
log.info(f"args: {vars(args)}")
```

[slide adapted from Evan Shelhamer]
Testing and debugging

debug with the default python debugger: **pdb**

```python
import pdb; pdb.set_trace()
```


[slide adapted from Evan Shelhamer]
Testing and debugging

**check gradients** using finite difference methods

- [gradcheck](#) is the checker bundled into PyTorch
- [cs231](#) has gradient checking rules of thumb
- [Tim Vieira](#) has further tips for accurate and thorough checking

[slide adapted from Evan Shelhamer]
more hardware, more problems don’t parallelize immediately

• make your model work on a single device first

• attempt to parallelize on a single machine

• only then go to a multi machine set

• and check that iterations/time actually improves

see Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour for good advice
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