Intermediate pytorch concepts

Alberto TONDA, Ph.D. (Senior permanent researcher, DR)

UMR 518 MIA-PS, INRAE, AgroParisTech, Université Paris-Saclay
UAR 3611, Institut des Systèmes Complexes de Paris Île-de-France

Outline

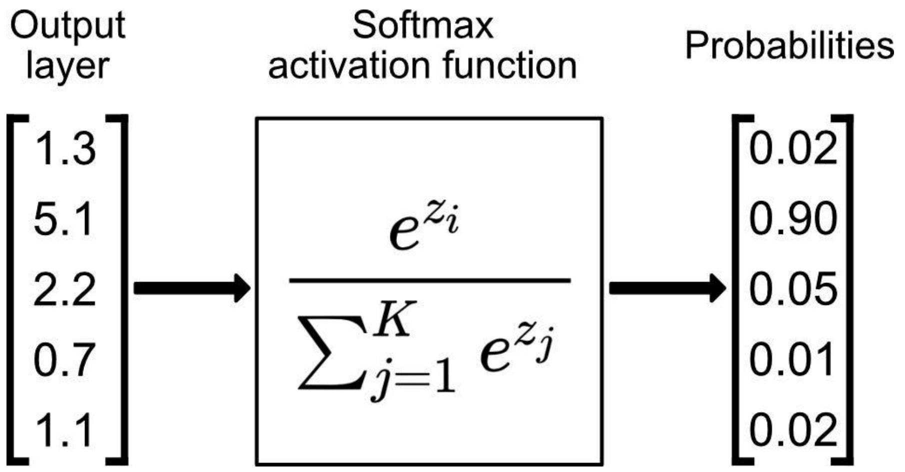
- Where is the SoftMax?
- Monitor performance
- Tensorboard
- Stochastic Gradient Descent
- Activation functions
- Checkpointing

TOP 10 DEEP LEARNING FRAMEWORKS

10. You can't
9. Rank them
8. Because each has
7. Their own merits
6. That make them better
5. Tools for certain tasks
4. Than the others
3. Just appreciate that they're
2. All used to build great stuff
1. Pytorch

Where is the SoftMax?

- We grazed over classification
  - But in literature, output tensor is sent through SoftMax
  - SoftMax is used to get values in [0.0,1.0] who add to 1.0
  - Sometimes called “class probabilities”, but **they are not**
- Where was the SoftMax? Was there an error in the code?



Where is the SoftMax?

- The SoftMax is *inside* the loss function

CROSSENTROPYLOSS

CLASS torch.nn.CrossEntropyLoss(*weight=None*, *size_average=None*, *ignore_index=-100*, *reduce=None*, *reduction='mean'*, *label_smoothing=0.0*) [SOURCE]

This criterion computes the cross entropy loss between input logits and target.

It is useful when training a classification problem with C classes. If provided, the optional argument `weight` should be a 1D *Tensor* assigning weight to each of the classes. This is particularly useful when you have an unbalanced training set.

The *input* is expected to contain the unnormalized logits for each class (which do *not* need to be positive or sum to 1, in general). *input* has to be a Tensor of size (C) for unbatched input, $(minibatch, C)$ or $(minibatch, C, d_1, d_2, ..., d_K)$ with $K \geq 1$ for the *K*-dimensional case. The last being useful for higher dimension inputs, such as computing cross entropy loss per-pixel for 2D images.

Where is the SoftMax?

- What is a *logit*?!?

n the unnormalized logits for each class (

or of size (C) for unbatched input. $(mi$

Where is the SoftMax?

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- What is a *logit*?!?

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Probit model

Article Talk

From Wikipedia, the free encyclopedia

In statistics, a **probit model** is a type of regression where the dependent variable can take only two values, for example married or not married. The word is a portmanteau, coming from ***probability* + *unit***.[1] The

In 1934, Chester Ittner Bliss used the cumulative normal distribution function to perform this mapping and called his model probit, an abbreviation for "**prob**ability un**it**". This is, however, computationally more expensive.[2]

In 1944, Joseph Berkson used log of odds and called this function *logit*, an abbreviation for "**log**istic un**it**", following the analogy for probit:

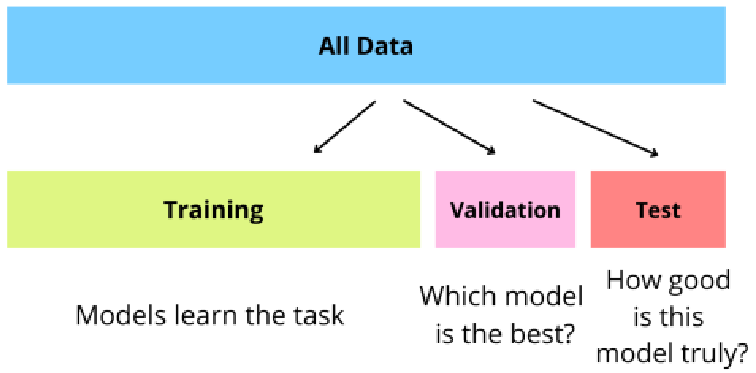
> "I use this term [logit] for $\ln p/q$ following Bliss, who called the analogous function which is linear on x for the normal curve 'probit'."
>
> —Joseph Berkson (1944)[3]

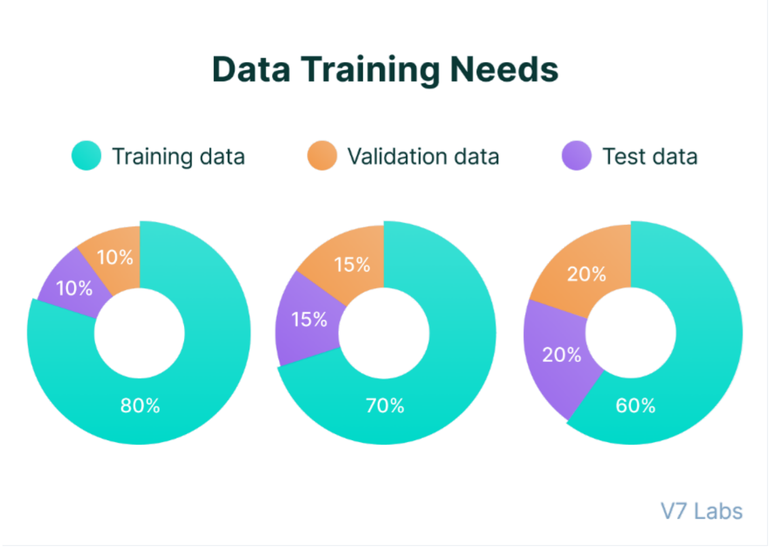
Monitor performance

- Assess performance during training
  - But performance is better evaluated on **test**!
  - Evaluating performance on training is not very informative
  - Overfitting gives the illusion of increasing performance on training
- We want to know performance on *unseen* data!
- But at the same time, we don't want to use the test set!
- How can we solve this conundrum?

Monitor performance

- Further split in the data
  - Three parts: training, **validation**, test
  - Validation is used to assess performance at a given epoch
  - Commonly called “validation loss” (vs “training loss”)





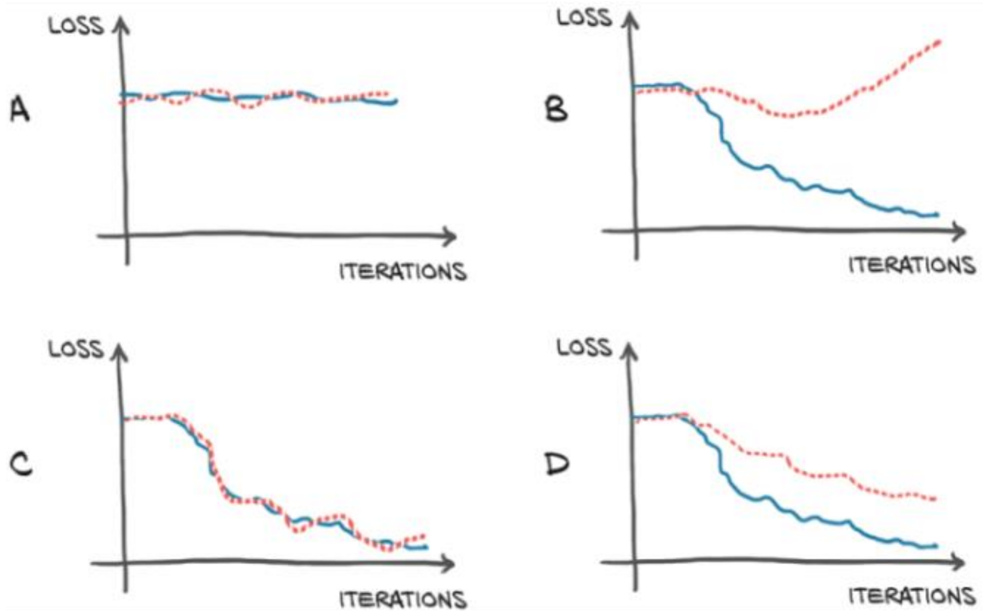
Monitor performance

- Using training loss and validation loss, **detect overfitting**!
  - How?

Monitor performance

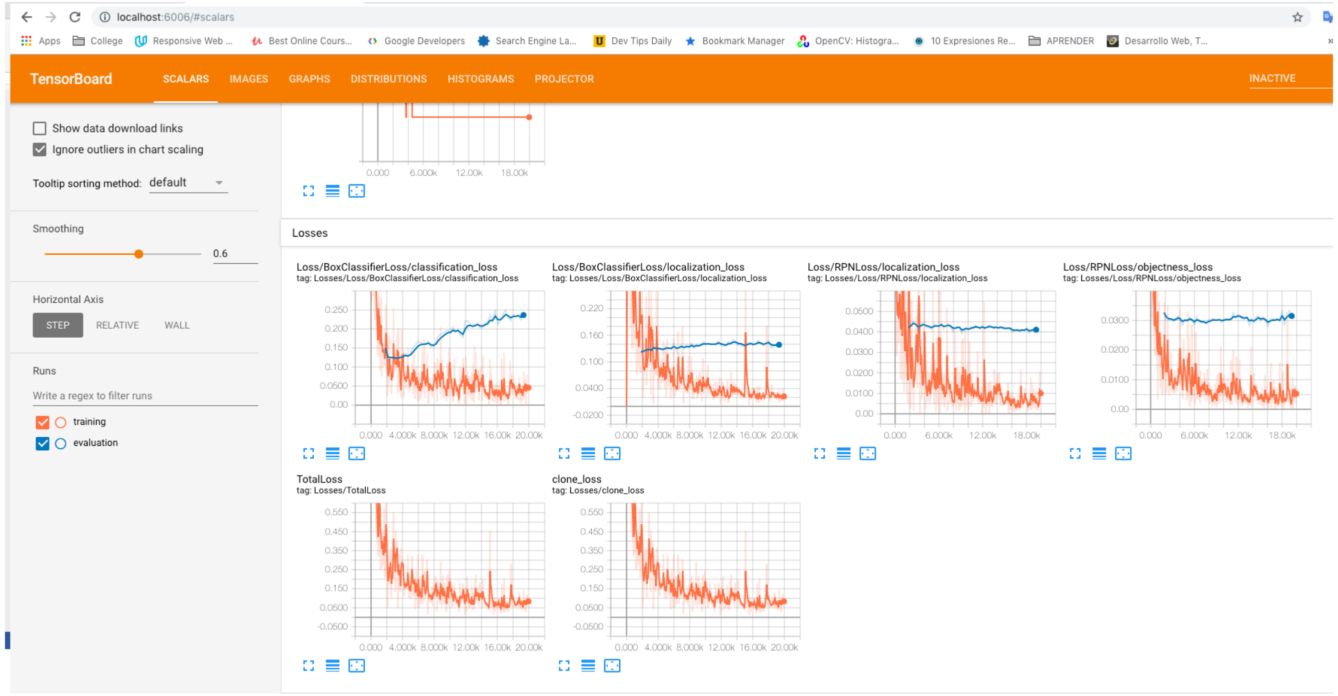
- Using training loss and validation loss, **detect overfitting**!
  - When training loss keeps decreasing, but validation loss *increases*
  - …or remains stationary for a long time

Training loss
Validation loss



Tensorboard

- Software developed by Google (part of Tensorflow)
  - During training, write logs to text files
  - Read text files and present a visualization

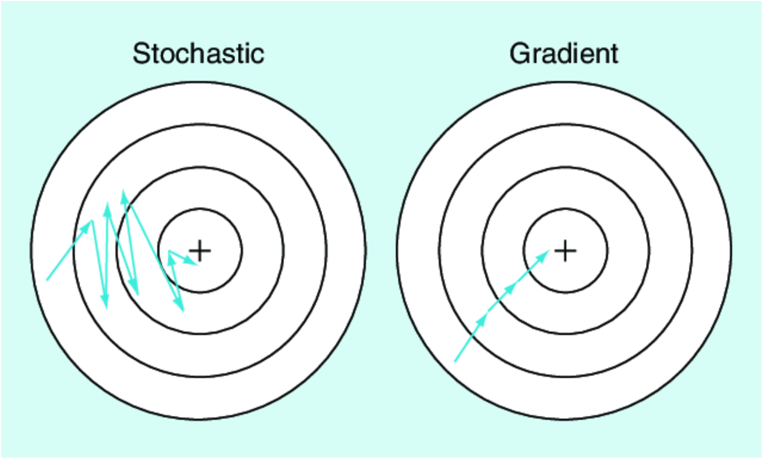


Stochastic Gradient Descent?

- You already used SGD in the exercises
- What is *stochastic* about SGD?

(Really) Stochastic Gradient Descent

- It was NOT STOCHASTIC AT ALL!
- Difference between SGD and GD
  - SGD updates gradients after seeing a *random subset* of the data
  - Random subset is called **batch**
  - Smaller, more frequent updates are more robust and *faster*
  - Typically SGD uses a **smaller learning rate**



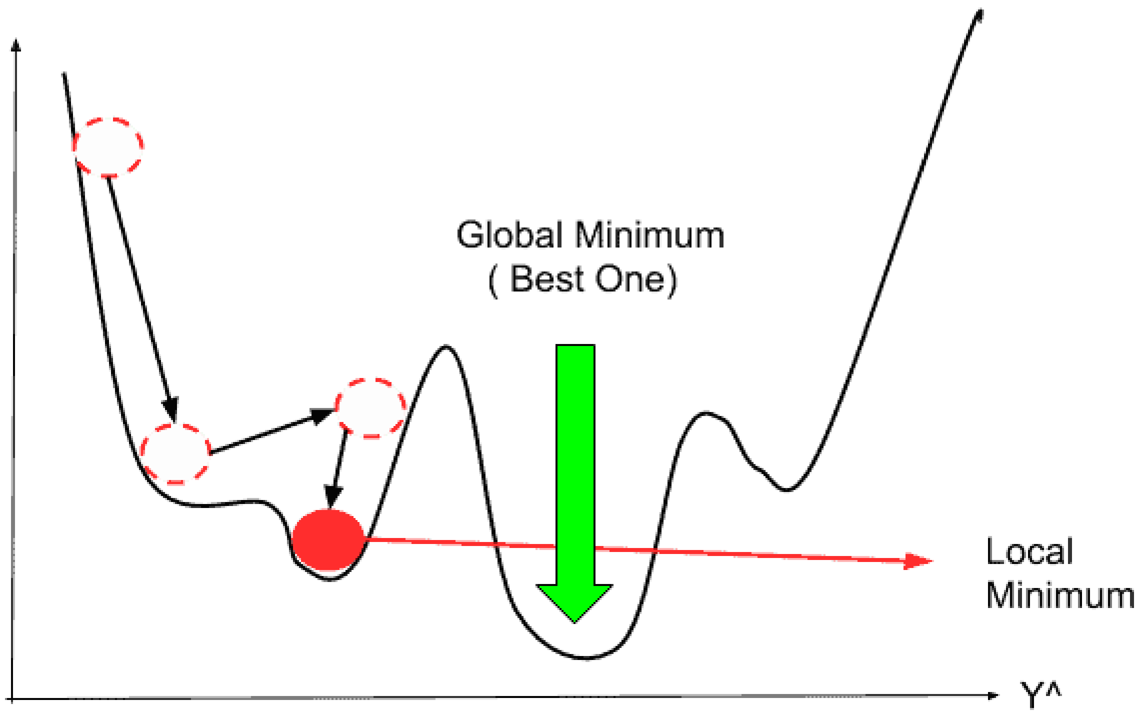
Beyond Stochastic Gradient Descent

- Nobody uses SGD anymore
  - However, its descendants thrive!
  - A cumulative research effort over generations to overcome issues

- Issues of gradient-based techniques
  - Hard/impossible to get out of local optima
  - Starting point of exploration matters
  - Step size? Too small / too large leads to convergence issues

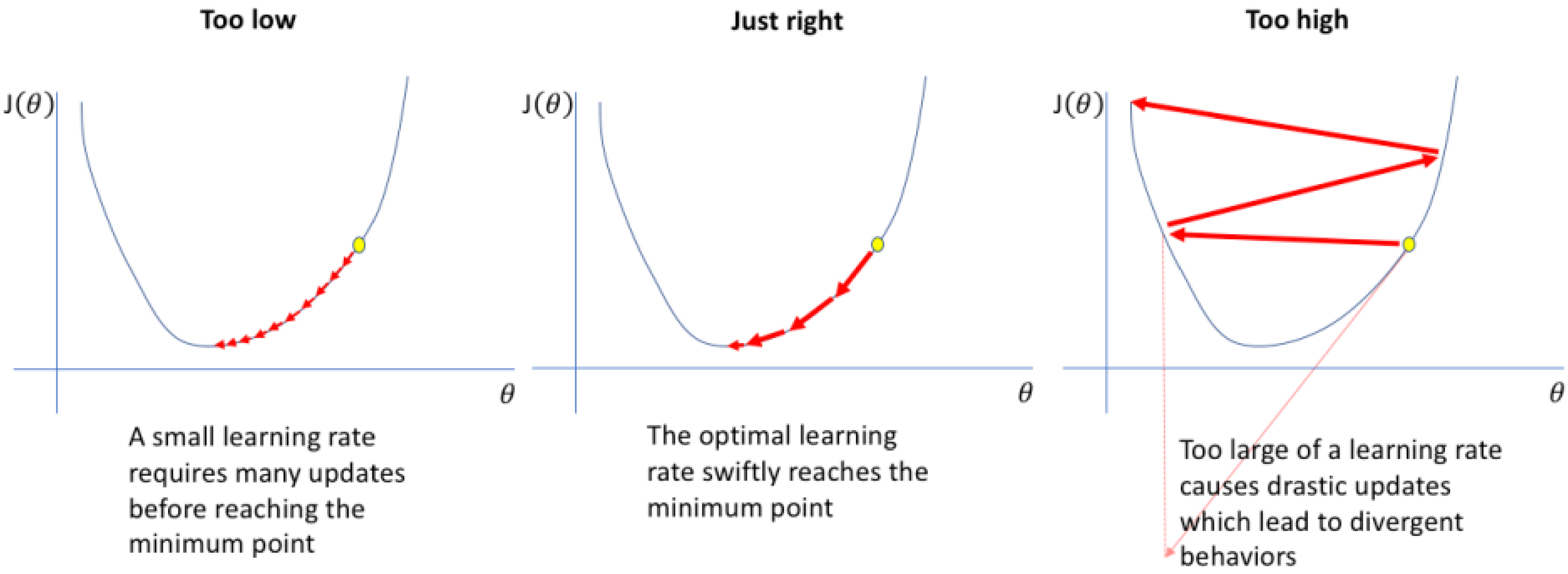
Issues with gradient-based techniques

- Starting point of exploration matters



Issues with gradient-based techniques

- Step size? Too small / too large lead to convergence issues



Modern gradient-based techniques

- Momentum

$$\mathbf{v}^{(k+1)} = \beta\mathbf{v}^{(k)} - \alpha\mathbf{g}^{(k)}$$
$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{v}^{(k+1)}$$

  - Accumulates "velocity" like a ball rolling down an incline
  - Much faster at traversing nearly flat areas of search space
- However, it adds an extra parameter (α, β)
  - α is still the learning rate
  - β represents the importance given to velocity during update

Modern gradient-based techniques

- However, now it cumulates *too much* momentum!
- Nesterov momentum

$$\mathbf{v}^{(k+1)} = \beta \mathbf{v}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)} + \beta \mathbf{v}^{(k)})$$
$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{v}^{(k+1)}$$

  - Evaluate the gradient at the point planned to end in
  - Velocity is rescaled accordingly

Modern gradient-based techniques

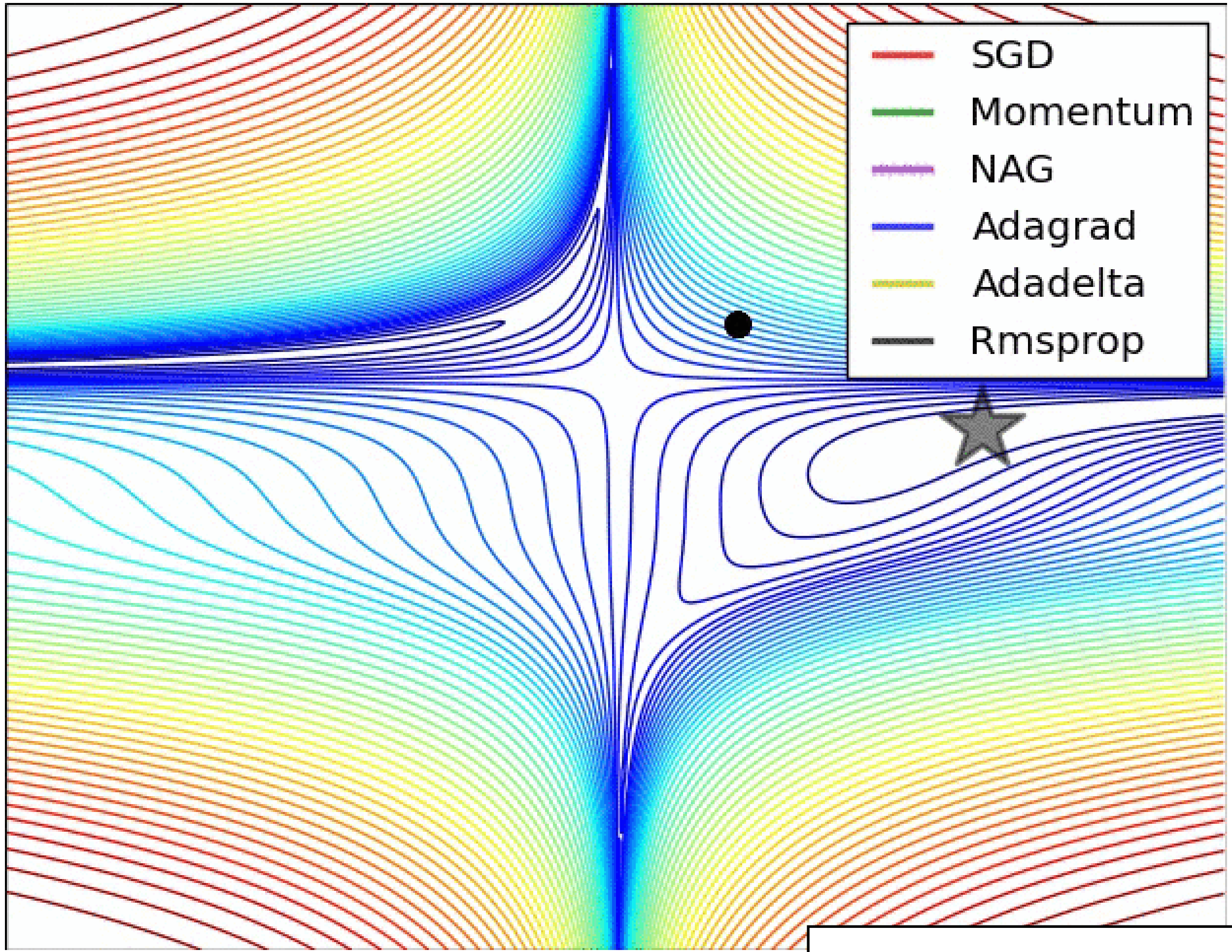
- Further issues motivated further advances (**Adagrad**)
  - The step size could be different in each dimension
  - Maintain a “memory” of the gradient values in each direction

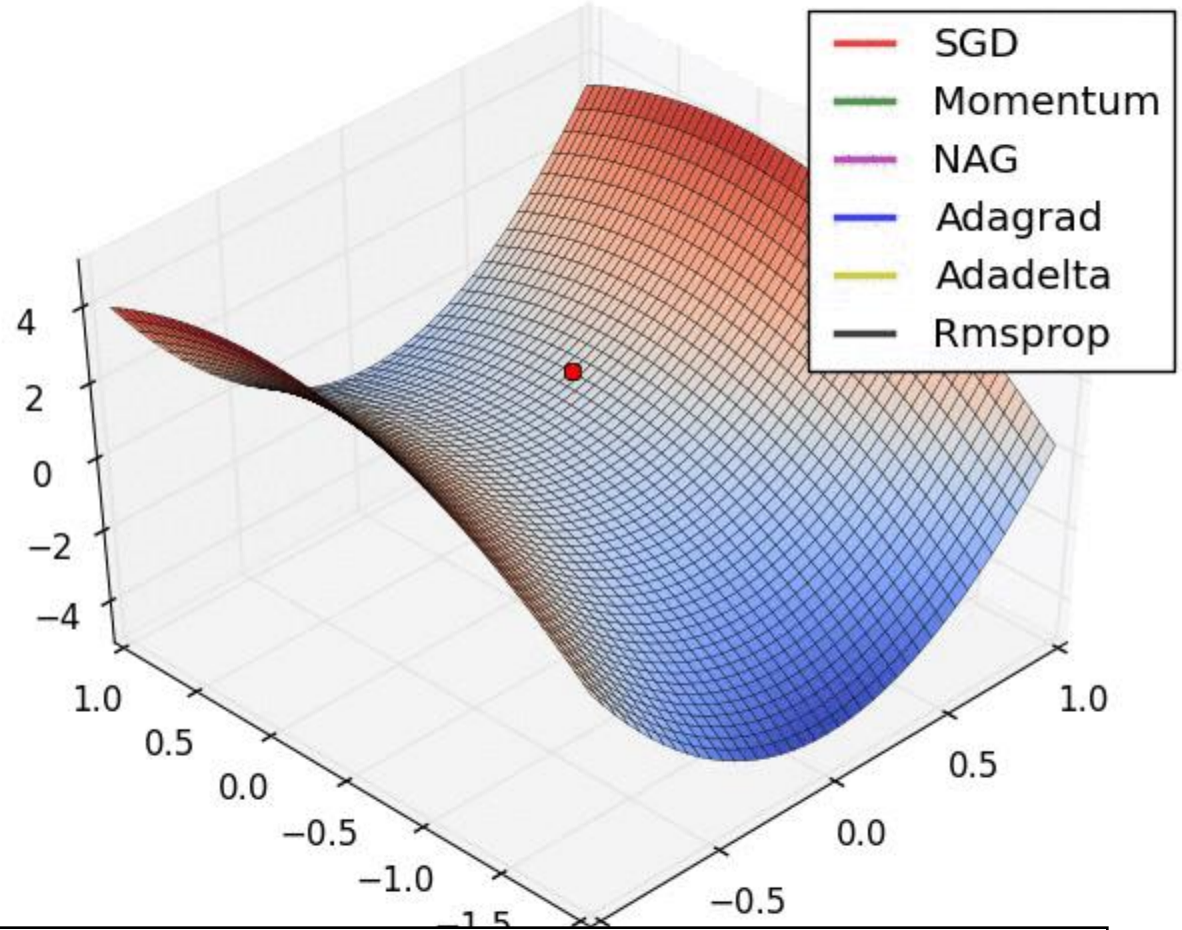
$$x_i^{(k+1)} = x_i^{(k)} - \frac{\alpha}{\epsilon + \sqrt{s_i^{(k)}}} g_i^{(k)}$$

$$s_i^{(k)} = \sum_{j=1}^{k} \left(g_i^{(j)} \right)^2$$

  - However, this leads to the step size always decreasing

Modern gradient-based techniques





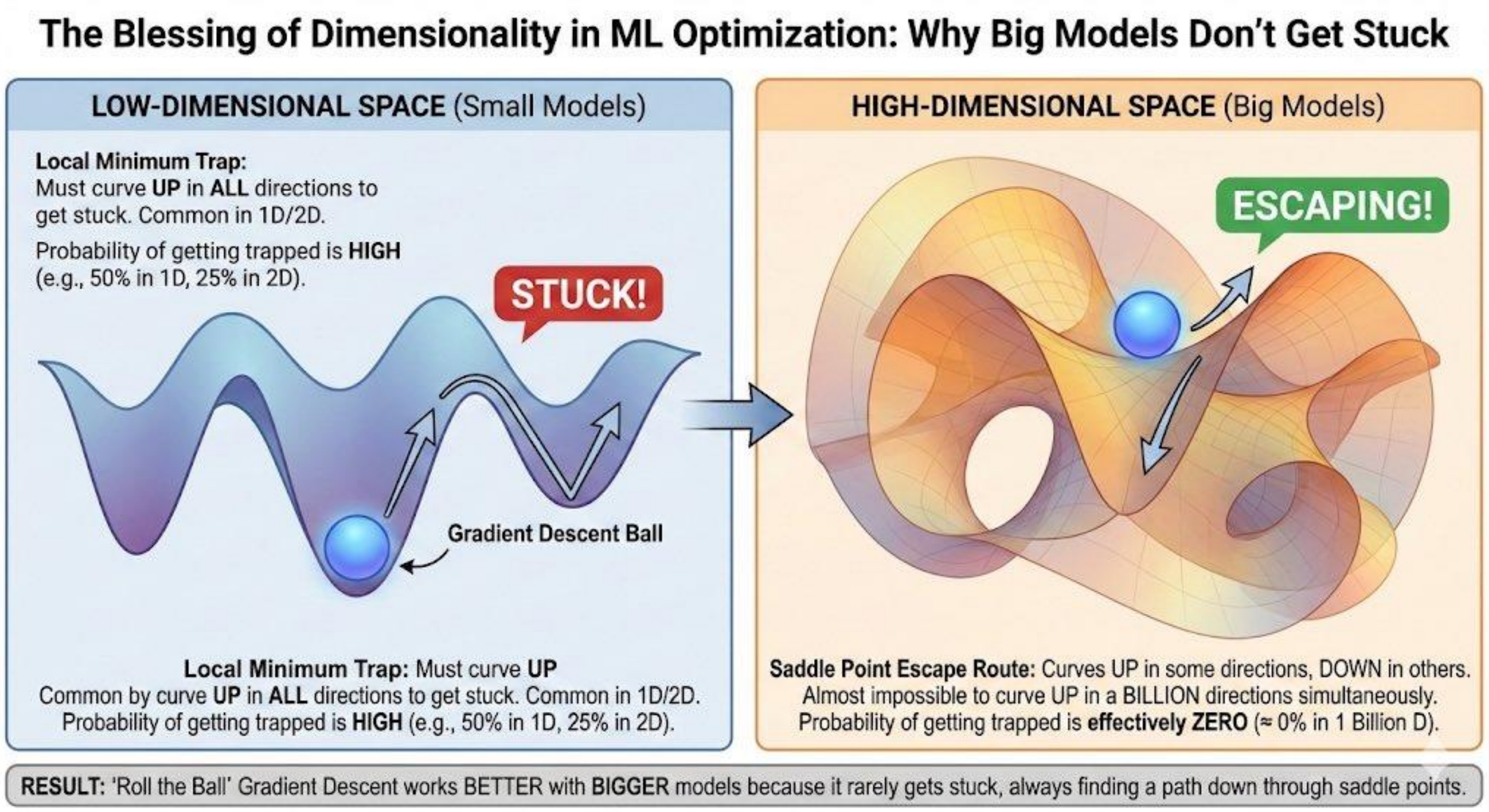
https://deepdatascience.wordpress.com/2017/02/03/optimiser-choice/

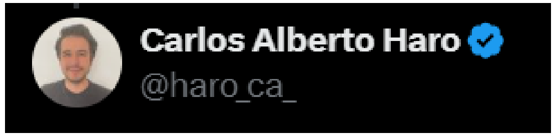
Modern gradient-based techniques

- Solutions to issues of previous algorithms create new issues
  - Commonly used **Adam** and **RMSProp** have 3-4 hyperparameters
  - Also take more memory (history of gradient values)
  - Default values work reasonably well (but not always)

- Practical advice
  - Use **Adam** (Adaptive Moment Estimation) in most cases
  - Check out new algorithms! torch.optim.*

Why does SGD work?





torch.utils.data.Dataset

- Class to manage loading and fetching samples in datasets

```python
# here is our new class, inheriting from Dataset; it is supposed to be a generic
# class to load data sets obtained from openml
class OpenMLDataset(torch.utils.data.Dataset) :

  # we create our own builder, that has two compulsory arguments, X (tensor with feature values)
  # and y (tensor with values of the target)
  def __init__(self, X, y) :
    # call __init__ of the parent class (in this case, the parent class has no __init__, but this is an implementation detail)
    super(OpenMLDataset, self).__init__()
    # we store the information internally in the object, as two attributes self.X and self.y
    self.X = X
    self.y = y

  # the function that returns the total number of samples is easy
  def __len__(self) :
    return self.y.shape[0]

  # the function that gets a single sample is also pretty straightforward
  def __getitem__(self, index) :
    return self.X[index], self.y[index]
```

Schedulers

- Adapt optimizer hyperparameters **during training**?
  - Especially learning rate!
  - In general, large(r) initial learning rate, small(er) at the end
  - “Exploration vs Exploitation”
- Example: torch.optim.lr_scheduler.ExponentialLR
  - All hyperparameters, epoch k: $h^{(k+1)} = h^{(k)} \cdot \gamma; \gamma < 1.0$
  - In practice, all hyperparameter values slowly become smaller
  - Common values: $\gamma = 0.9, \gamma = 0.99$
- Other ideas: torch.optim.lr_scheduler.*

Pseudo-random number generation in pytorch

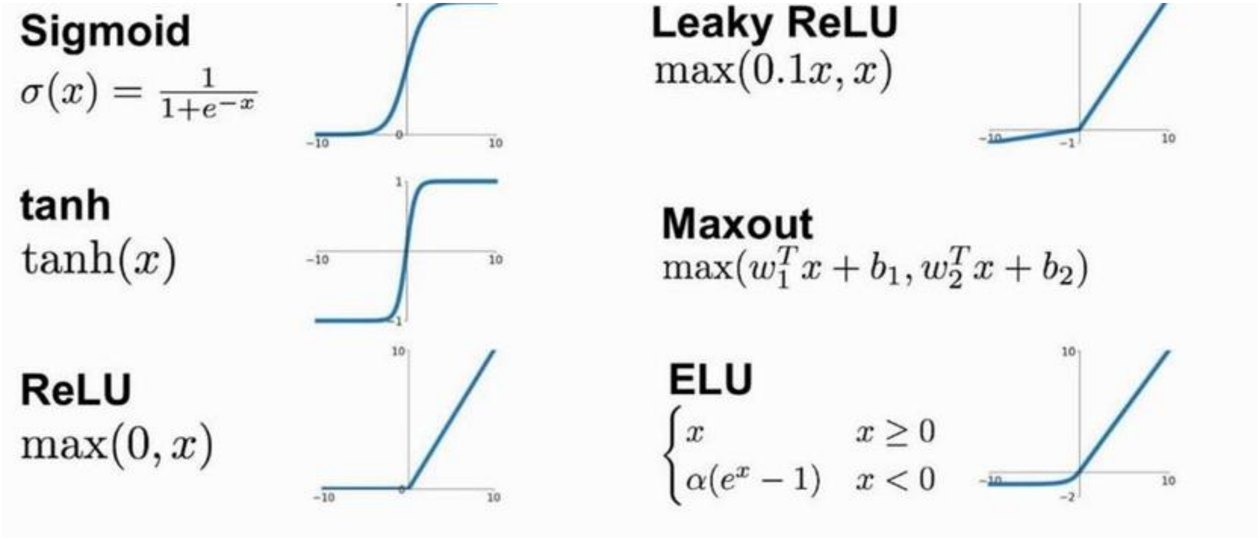
- Unfortunately, it's not easy
  - Computing on GPUs makes consistent PRNG difficult
  - Libraries optimized for *speed*, not consistent behavior

- Still, good practices:

  https://pytorch.org/docs/stable/notes/randomness.html

Activation functions

- So far, we used one of the most basic activation functions
  - But there are several others, more modern
  - Better theoretical properties and empirical results



Activation functions

- Practical advice
  - Check function typically used in literature for target application
  - For recurrent neural networks, TanH or Sigmoid
  - When in doubt, go for ReLUs

- Lots of available activation functions
  - https://pytorch.org/docs/stable/nn.html#non-linear-activations-weighted-sum-nonlinearity
  - https://pytorch.org/docs/stable/nn.html#non-linear-activations-other

Checkpointing

- Training neural networks can take a long time
  - We can **save the state of the network** during training!
  - State depends only on weight values (+ optimizer, + scheduler)
  - Stop and resume training
  - **Share weights** with other people!

- Checkpoints are one of the foundations of **transfer learning**

Questions?

Bibliography

- pytorch FAQs, https://pytorch.org/docs/stable/notes/faq.html