Training
Deep Learning models

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Agenda for today

- Recap from yesterday: what have we learned?

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- Training neural network

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- First deep learning model

Quick recap

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- They are highly nonlinear
- They are highly flexible
- We went over the concepts of weights, layers and activation functions
- We created a tight link with the field of statistics

Training neural networks

Numerical computation in general

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- Solve mathematical problems by updating the estimates of the solution via an iterative process - a recipe.
- It all boils down to what computers can do best: compute, fast.
- Deep learning algorithms require high amount of numerical computation.
- Mainly because we can't close-form solve complicated, realistic problems.

A stroll down memory lane: derivatives

- If $z = f(y)$, the derivative $f'(y) := \frac{dz}{dy}$ helps us figure out how much the output of the function should change with a small (infinitesimal) ε nudge to the parameter y, i.e $f(y+\varepsilon) \approx f(y) + \varepsilon f'(y)$.

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- A gradient is a general notion of derivative when there is a vector of parameters (rather than a scaler).
- For no special reason other than mathematical convention we use the notation of partial derivative with respect to each parameter like so

$$f'(parameter_i) := \frac{\partial function}{\partial parameter_i}.$$

A stroll down memory lane: chain rule

- We use the chain rule of calculus. If $y = g(x)$ and $z = f(g(x)) = f(y)$ then the derivative of z with respect to x is given by
$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

- In our context: the impact off parameter i on the loss function is found by first finding the impact of the activation function on the loss function and then the impact of the of the parameter on the activation function.

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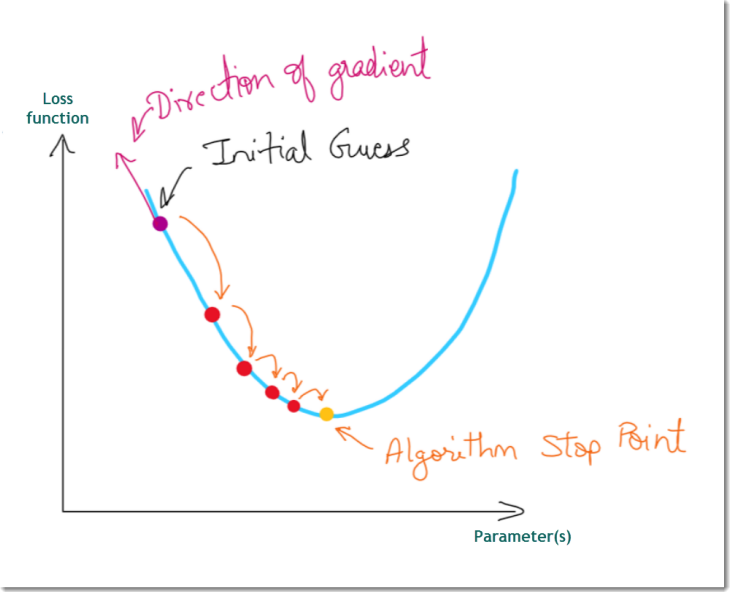
- Gradients make it easy for us to find a good solution.
- The good solutions are just that. Good, but not optimal in any sense.
- Over the years researchers found new tricks to progress faster towards a solution.

Enter: gradient based optimization

Intuition


Direction of gradient
Loss function
Initial Guess
Algorithm Stop Point
Parameter(s)

(batch) Gradient descent

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla_{\mathbf{w}} \mathcal{R}(\mathbf{w})$$

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  Reminder: $\mathcal{R}(\mathbf{w}) = \mathrm{E}\left(\mathcal{J}(\mathbf{w})\right) = \mathrm{E}(\frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\widehat{y}_i, y_i))$. Finally, $\nabla_{\mathbf{w}}$ denotes the gradient (the vector of partial derivatives. Each partial derivative with respect to a particular weight/parameter).
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- Why the minus in the formula?

(batch) Gradient descent (continued)

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- Each "nudge" requires computation of the entire data for evaluating $\nabla_{\mathbf{w}} \mathcal{L}(\widehat{y}_i, y_i)$. This is known as *batch* gradient descent.
- Note that $\widehat{y}_i$ is a function of the input $\mathbf{x}$ and of course the weights $\mathbf{w}$. In our text book they use (adhering to their notation) they use the more exhaustive

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{x}^{(i)}, y^{(i)}, \boldsymbol{\theta}\right)$$

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- Enter *stochastic gradient descent*.

Stochastic gradient descent

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- Easy. Pick a data point at random and update the weight vector based on the gradient with all calculation based on that data point only.

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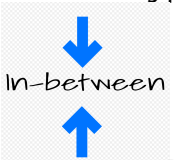
- Direction of update not very stable though. Teaser: what influence the stability of this choice? for which data this choice is ok, and for which it is unwise?
- We have seen *batch* and *stochastic*. Typically we choose something



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- More computationally efficient than the batch gradient descent, and not as noisy as the fully stochastic version.
- The size of the mini-batch is another hyper-parameter to consider.
- In both stochastic and mini-batch version of the algorithms we pass through all the data. However, the mini-batch version benefits for algebraic practical implementation (vectorization) which allows gradient computing in parallel.

Minibatch size, and few comments

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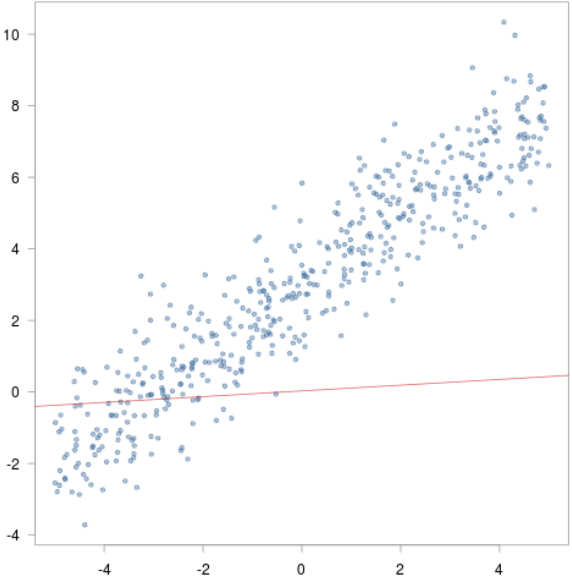
- The specialized language is a bit confusing. I would not use the word "batch" to indicate that the whole sample is used +, minibatch is also a stochastic algorithm. However, we (you) should adhere to the convention.

Numerical computation - putting it all together

1. Initialize the weights.
2. Forward propagate: the inputs from a training set are passed through the neural network and an output is computed.
3. You define an error function. It captures the difference between the actual output and your model's output, given current model weights.
4. Backpropagation - change the weights for the neurons, in order to reduce the error.
5. Update - weights are changed according to the results of the previous step.
6. **Iterate** - because the weights are only nudged at each step, many iterations are required in order for the network to learn. The amount of iterations needed to converge depends on the learning rate, the network architecture, and the specific optimization method used.

Illustration:



Accelerated gradient methods

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- Over time researchers found ways to speed up the convergence towards a solution.
- We now review few seminal contributions.

Learning rate decay

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- Start with large steps and decrease them over time.
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- Same step size for all parameters (still).

Gradient descent with momentum

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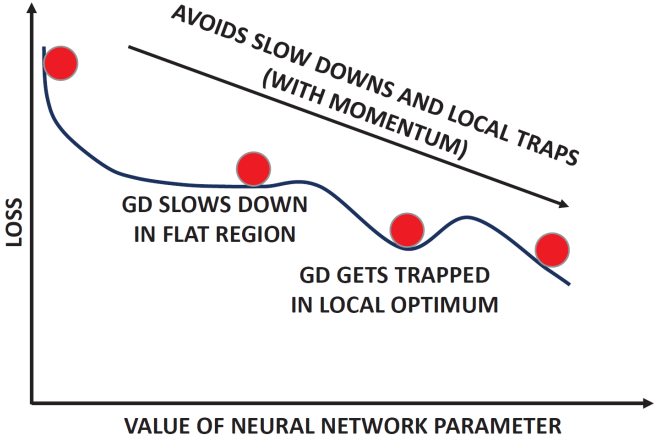
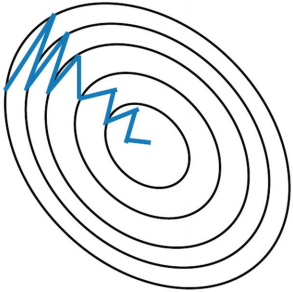
- But we can do better.
- We now explain the intuition behind adjusting the learning rate based on momentum.

Gradient descent with momentum (continued)



Gradient descent with momentum (continued)

Stochastic Gradient Descent **withhout** Momentum



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- We give preference to direction where change is consistent.
- Opposite changes cancel each other in the moving average calculation.
- Implication: less zig-zagging.

Gradient descent with momentum (continued)

How does it work?

- Instead of simply updating:

$$\mathbf{w}_{k+1} = \mathbf{w}_t - \eta \nabla_{\mathbf{w}} \mathcal{L}$$

We now use

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \nu_{k+1},$$

where

$$\nu_{k+1} = \beta \nu_k + \eta \nabla_{\mathbf{w}} \mathcal{L}$$

Note I have remove dependency on data and parameters in the loss function, to ease readabiliy

Gradient descent with momentum (continued)

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- A nice reference here (but also nice in general) is Hinton 2012.

Adagrad

- Adding some friction: use the squared, element-wise, derivatives as a way to adjust the learning rate. Slow down if the speed is "too fast", and increase speed when it's "too slow".

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$$w_{k+1,i} = w_{k,i} - \eta \frac{\nabla_{\mathbf{w}} \mathcal{L}_i}{\sqrt{\tilde{\nu}_{k,i} + \varepsilon}},$$

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- $\tilde{v}$ to make it differentiate it from this v notation we used for momentum.

What is the problem with this algorithm?

RMS (Root Mean Square) prop*

The most straight forward extension for Adagrad you can think of.

- Before (with Adagrad):

$$\tilde{v}_i = \sum_{j=1}^{k} \left(\frac{\partial \mathcal{L}}{\partial w_i} \right)_j^2$$

"slide 29 in lecture 6"

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- Before (with Adagrad):

$$\tilde{v}_i = \sum_{j=1}^{k} \left(\frac{\partial \mathcal{L}}{\partial w_i} \right)_j^2$$

- Now, forget iteration which are too far back:

$$\tilde{v}_{k+1,i} = \tilde{\beta} \tilde{v}_{k,i} + (1 - \tilde{\beta}) \left(\frac{\partial \mathcal{L}}{\partial w_i} \right)_{k+1}^2$$

"slide 29 in lecture 6"

Adam - adaptive moment estimation

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  where we now have both ν and $\tilde{\nu}$ involved.
- A most popular variant.

Numerical prompts

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- Gradient Checking.

Next topic of today:

Regularization

Regularization as a concept

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- Instead of trying to be right on the first go, we overshot and scale back complexity.
- There are many strategies to do that.
- A good regularizer $\Rightarrow$ <u>reduces variance</u> without increasing bias, much.

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- Why regularization helps us?
  - Prevents model's over-flexibility $\Rightarrow$ less expressive
  - Equivalent to "contaminating" the training data (helping us to generalize on new data).

Bias variance tradeoff

The MSE can be decomposed like so:

$$\mathcal{MSE} = \mathcal{E}_x \left\{ \text{Bias}_{\mathbf{w}}[\hat{f}(x; \mathbf{w})]^2 + \text{Var}_{\mathbf{w}}[\hat{f}(x; \mathbf{w})] \right\} + \sigma^2$$

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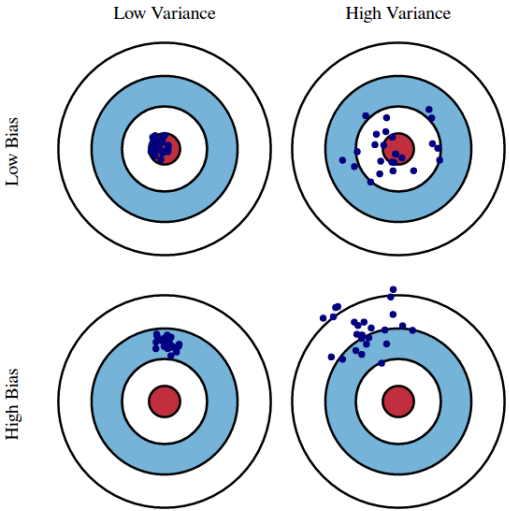
- We can't do anything about σ^2
- We can trade bias for variance. And more relevant: the reverse.

Bias variance tradeoff



We now review few ways to regularize deep learning models

Regularization - Data augmentation

- A paradigm shift from old-school econometrics.

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- Rotate the data.
- Add data which was generated synthetically.

Regularization - norm restrictions

$$\tilde{\mathcal{L}}(\mathbf{w}; \boldsymbol{X}, \boldsymbol{y}) = \mathcal{L}(\mathbf{w}; \boldsymbol{X}, \boldsymbol{y}) + \alpha\Omega(\mathbf{w}),$$

$\Omega(\cdot)$ is usually a quadratic norm penalty. E.g $\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2$. ($L^2$ regularization, or Tikhonov regularization).

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- Another common penalty is the L^1 regularization: $\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_1 = \sum_i |w_i|$

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$$\tilde{\mathcal{L}}(\mathbf{w}; \boldsymbol{X}, \boldsymbol{y}) = \mathcal{L}(\mathbf{w}; \boldsymbol{X}, \boldsymbol{y}) + \alpha\Omega(\mathbf{w}),$$

$\Omega(\cdot)$ is usually a quadratic norm penalty. E.g $\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2$. ($L^2$ regularization, or Tikhonov regularization).

- Another common penalty is the L^1 regularization: $\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_1 = \sum_i |w_i|$
- What is the difference?

Regularization - norm restrictions (continued)

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- $\alpha = 0 \quad \Rightarrow$ no regularization.
- We can keep $\alpha_l = \alpha$ (l for layer), but we don't have to.

Regularization - early stopping

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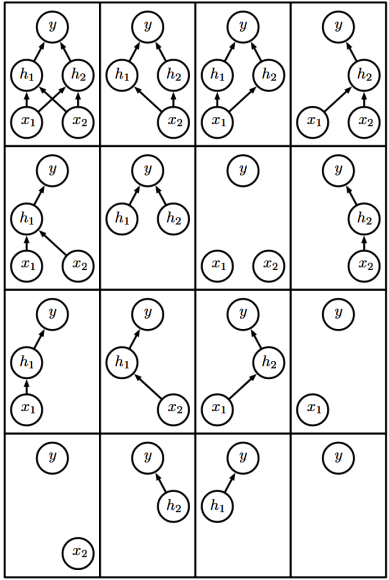
- If η is the learning rate and we have say τ training iteration then the product $\eta \times \tau$ is the effective capacity of the model.

Dropout

- Powerful regularization technique.



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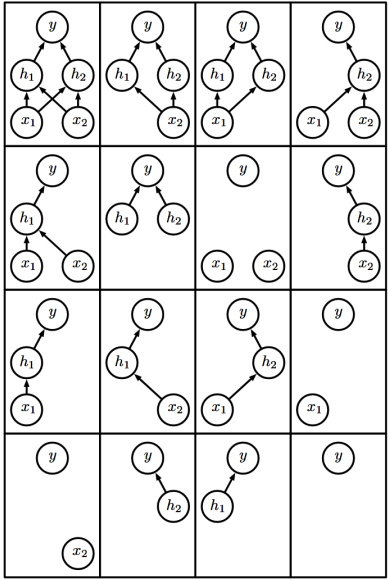
- Powerful regularization technique.
- Can be thought of as model averaging.



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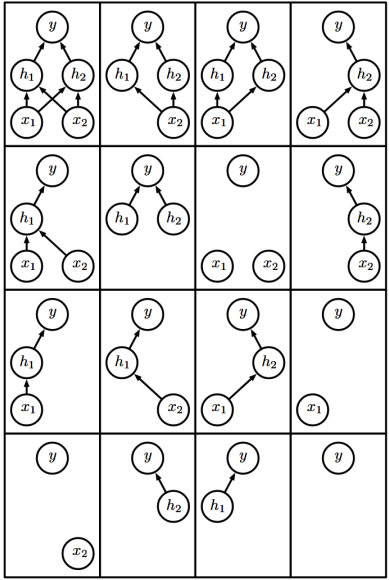

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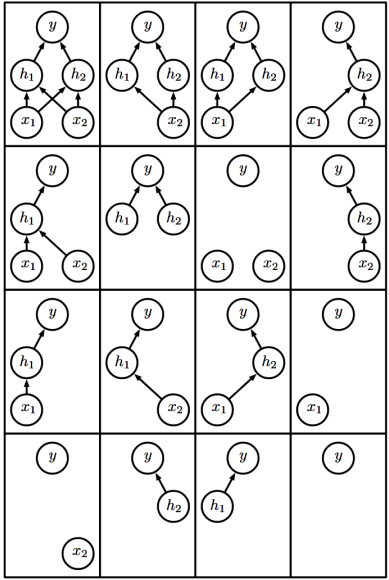
- Can be thought of as model averaging.
- The weights can't "rely" on inputs to be there.
- The probability of masking a neuron doesn't each layer.



Now Let's code!

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