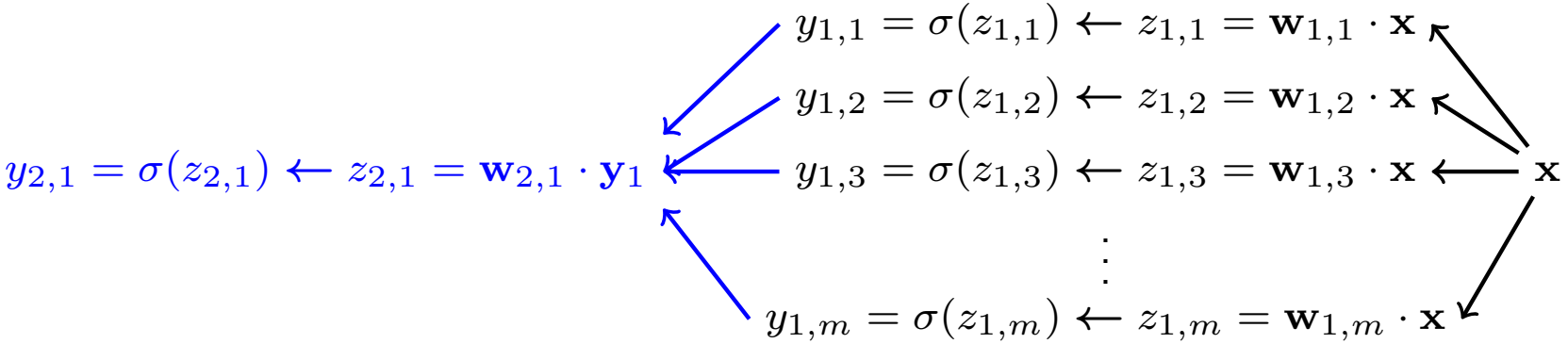
Neural Networks: Training and SGD

Spring 2021

Completing our matrix formalism



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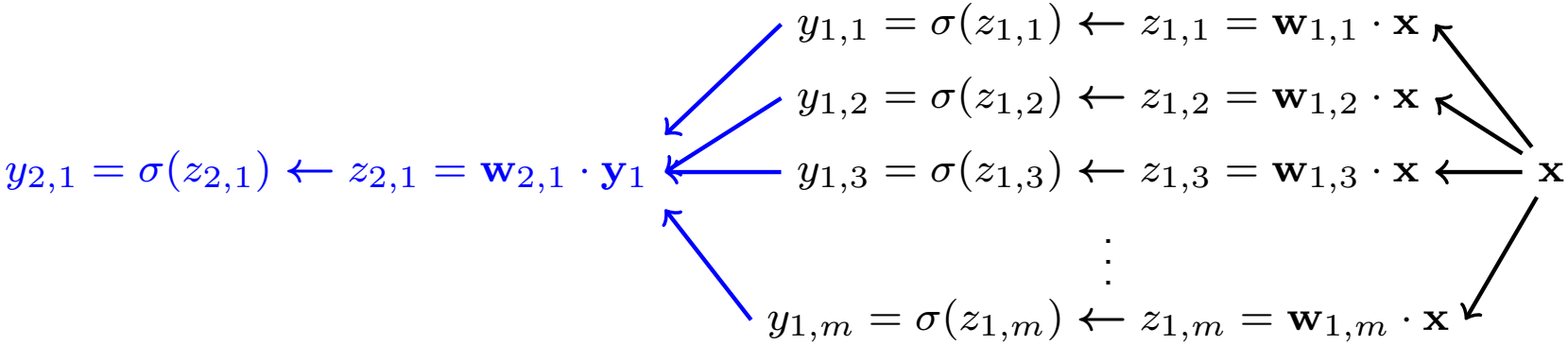

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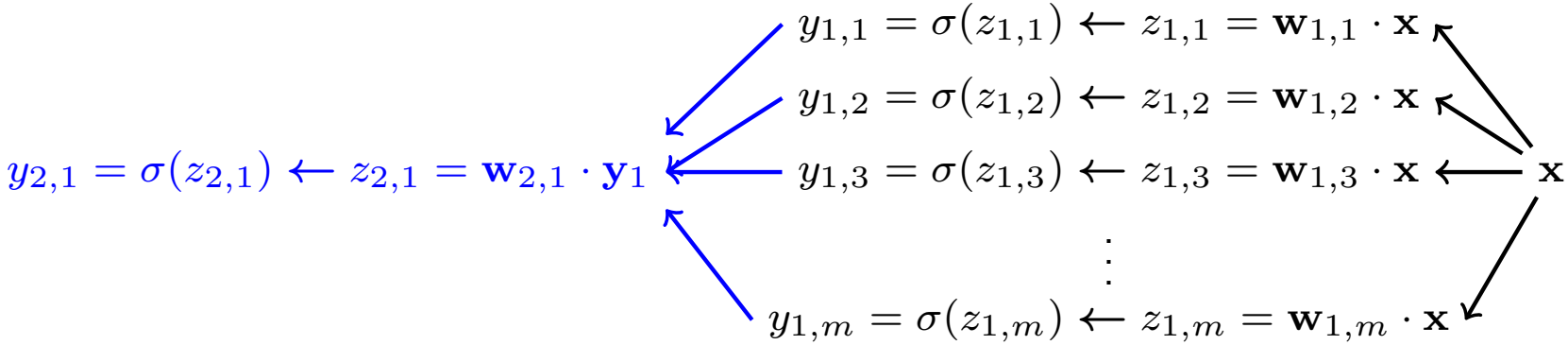

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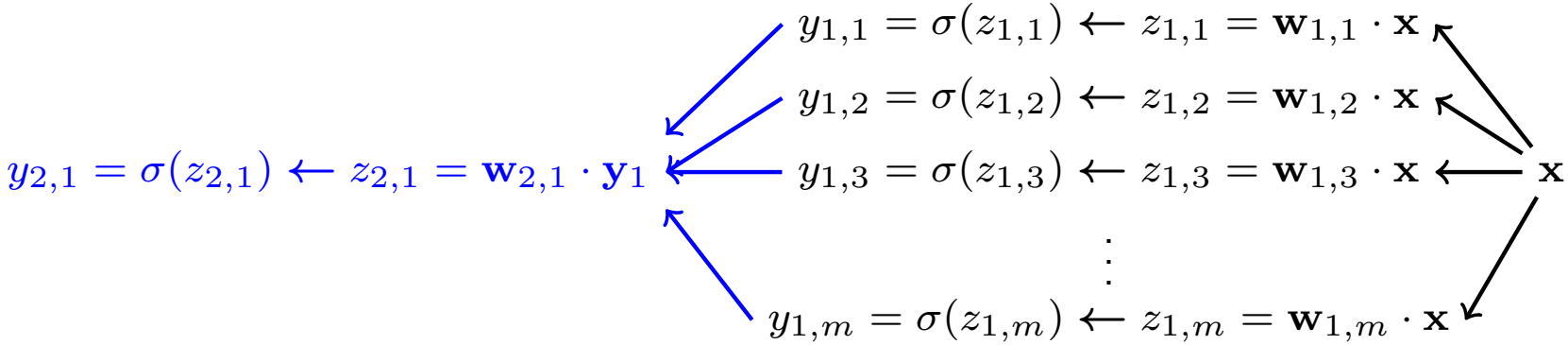

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In general, a network with d layers is

$$\mathbf{y}_d = \boldsymbol{\sigma}(\mathbf{W}_d(\boldsymbol{\sigma}(\mathbf{W}_{d-1}(\cdots\boldsymbol{\sigma}(\mathbf{W}_2(\boldsymbol{\sigma}(\mathbf{W}_1\mathbf{x})))))))).$$

Training neural networks

We need two things to train neural networks:

1. loss function L that measures how well the output of the final layer (y_d) compared with known training data.
2. A set of training data $(\mathbf{x}_i, y_i^{\text{true}})$.

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The loss function depends on all the weights in the network, i.e. $L_i(\mathbf{W}_d, \mathbf{W}_{d-1}, \ldots, \mathbf{W}_2, \mathbf{W}_1)$. We will abbreviate this as simply $L_i(\mathbf{W})$.

Gradient descent

We can use a gradient descent scheme to find the weights. Given an initial (random) set of weights $\mathbf{W}^{(0)}$:

1. Calculate the gradient of the *total loss*

$$\mathbf{g}(\mathbf{W}) = \sum_{i=1}^{N} \frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}.$$

2. Update the weights using

$$\mathbf{W}^{(1)} = \mathbf{W}^{(0)} - \alpha \mathbf{g}(\mathbf{W}^{(0)}).$$

3. Repeat.

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The problem is the gradient calculation.

- The gradient has one entry for each parameter, of which there are thousands!
- These computations are repeated over all N points in the dataset *for each iteration*!

Stochastic Gradient Descent (SGD)

- For neural network training we use an alternative to gradient descent called *Stochastic Gradient Descent*, or SGD.
- SGD alternates between forward and backward passes through the model.
- SGD updates parameters using the loss for a single point.
- A single point provides a noisy, or *stochastic* approximation to the true loss gradient, but it is far more efficient.

The SGD algorithm

1. Select a single training point $(\mathbf{x}_i, y_i^{\text{true}})$.
2. Make a **forward pass** through the model to compute the output of the neural network

$$y_{d,i} = \boldsymbol{\sigma}(\mathbf{W}_d(\boldsymbol{\sigma}(\mathbf{W}_{d-1}(\cdots\boldsymbol{\sigma}(\mathbf{W}_2(\boldsymbol{\sigma}(\mathbf{W}_1\mathbf{x}_i)))))))).$$

3. Compute the loss for this single prediction

$$L_i = (y_{d,i} - y_i^{\text{true}})^2.$$

4. Calculate the gradient at this point and the current weights.
5. Update the weights using

$$\mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} - \alpha\mathbf{g}(\mathbf{W}^{(k)}).$$

   This completes the **backward pass**.
6. Repeat for the next training point.

The SGD algorithm (simplified)

1. Select a single training point $(\mathbf{x}_i, y_i^{\text{true}})$.
2. Make a **forward pass** through the model to compute the output of the neural network
$$y_{d,i} \leftarrow \text{neural network} \leftarrow \mathbf{x}_i$$
3. Compute the loss for this single prediction
$$L_i \leftarrow (y_{d,i},\, y_i^{\text{true}})$$
4. Calculate the gradient at this point and the current weights.
5. Update the weights using
$$\frac{\partial L_i}{\partial \mathbf{W}} \rightarrow \mathbf{W}$$
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Implementing SGD

- Like gradient descent, SGD requires a step size hyperparameter (α).
- One pass through the entire training set is called an *epoch*.
- One epoch is not enough; often thousands are needed. The order of the training data is randomized between epochs.
- Some algorithms form *minibatches* by averaging a small number of training samples before updating the weights.

Why SGD?

- SGD is more efficient. Most datasets contain more points than are necessary to estimate the average, so computation is wasted.
- SGD is stochastic, just like the data. The stochasticity is a form of regularization.
- It just works, even if we don't understand why.

How do neural networks learn so well?

Neural network training *should* get stuck in local optima, but it doesn't. There are three theories why:

1. Lottery ticket theory: A good network is already somewhere in the randomly-initialized network.
2. There are no true local optima in high-dimensional spaces.
3. The noise in SGD allows training to "escape" local optima.

What else can we do to improve training?

1. **Regularize**. Neural networks can memorize anything, so we need to regularize them aggressively.
2. **Boosting**. Train in several rounds, weighting the loss function toward points that are not predicted correctly.
3. **Bagging**. Split the training data into parts and train a separate model on each part. Average the predictions of all the models.
4. **Experiment**. Change number and size of layers, hyperparameters, optimizers, batching, and regularization.

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4. Compute the loss

$$L(\mathbf{W}) = \left(\hat{Q}(s_i, a_i) - \widetilde{Q}(s_i, a_i; \mathbf{W})\right)^2.$$

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6. Go to #2 and repeat.

Deep Q-learning with terminal rewards

For games with only a terminal reward ($r_i = 0$ for $i \neq T$), we need to be careful in the near-terminal state:

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This reward will eventually be bootstrapped back through the Q-factors. However, we can speed up learning by setting

$$\hat{Q}(s_i, a_i) \approx r_T.$$

This rewards any state/action pair from games with a win and penalizes and state/action pair seen in losing games.

Summary

- Learning Q-factors is a dominant method for model-free RL.
- Q-factor estimates are updated by SARSA, Q-learning, or other algorithms.
- Q-factors can be tabulated for every state/action pair, or approximated with a parameterized function.
- Deep RL uses deep neural networks for Q-factor approximation.

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- Deep RL uses deep neural networks for Q-factor approximation.
- **Next time:** A "deeper" look at AlphaGo.