

This lecture covers

- Gradient descent
- Backpropagation
- Improved optimization: momentum, RMS-Prop, Adam
- Initialization
- Pragmatics of training neural networks
- Hyperparameter tuning

Gradient Descent

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- Neural networks do gradient descent with many parameters (variables) to minimize an error on a dataset. Some large language models have over 10^{12} parameters.

Two properties of differentiation are used in backpropagation:

- **Linear rule:** the derivative of a linear function, $aw + b$, is given by:

$$\frac{\partial}{\partial w}(aw + b) = a$$

- **Chain rule:** if g is a function of w and function f , which does not depend on w , is applied to $g(w)$, then

$$\frac{\partial}{\partial w} f(g(w)) = f'(g(w)) * \frac{\partial}{\partial w} g(w)$$

where f' is the derivative of f .

Use of chain rule

A network represents $f(e) = f_n(f_{n-1}(\dots f_2(f_1(x_e))))$, where example e has features x_e . Suppose $v_i = f_i(v_{i-1})$ and $v_0 = x_e$. Consider weight w used in the definition of f_j :

$$\begin{aligned} & \frac{\partial}{\partial w} \text{error}(f(e)) \\ &= \text{error}'(v_n) * \frac{\partial}{\partial w} f_n(v_{n-1}) \\ &= \text{error}'(v_n) * \frac{\partial}{\partial w} f_n(f_{n-1}(v_{n-2})) \\ &= \text{error}'(v_n) * f_n'(v_{n-1}) * \frac{\partial}{\partial w} (f_{n-1}(v_{n-2})) \\ &= \text{error}'(v_n) * f_n'(v_{n-1}) * f_{n-1}'(v_{n-2}) * \dots * \frac{\partial}{\partial w} (f_j(v_{j-1})) \end{aligned}$$

where f_i' is the derivative of f_i with respect to its inputs.

Backpropagation

- Backpropagation implements (stochastic) gradient descent for all weights.
- Two passes:
 - ▶ Prediction: given inputs compute outputs of each layer
 - ▶ Back propagate: Going backwards,

$$error'(v_n) * \prod_{i=0}^k f'_{n-i}(v_{n-i-1})$$

for k starting from 0 are computed and passed to the lower layers. Weights in each layer are updated.

functions is the list of functions that compose the neural network.

- 1: **repeat**
- 2: *batch* := random sample of *batch_size* examples
- 3: **for each** example *e* in *batch* **do**
- 4: **for each** input unit *i* **do** $values[i] := X_i(e)$
- 5: **for each** *fun* in *functions* from lowest to highest **do**
- 6: $values := fun.output(values)$
- 7: **for each** output unit *j* **do**
 $error[j] := \phi_o(values[j]) - Y_s[j]$
- 8: **for each** *fun* in *functions* from highest to lowest **do**
- 9: $error := fun.Backprop(error)$
- 10: **for each** *fun* in *functions* that contains weights **do**
- 11: $fun.update()$
- 12: **until** termination

Neural-network learner

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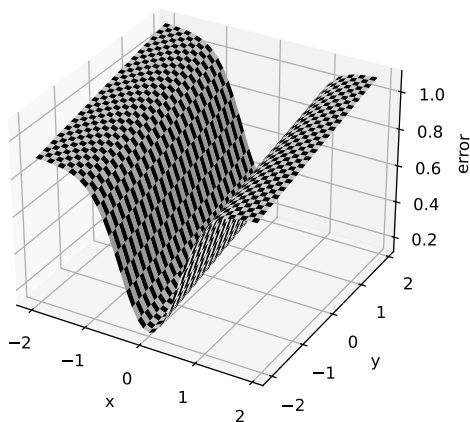
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Dense linear function

```
1: class Dense( $n_i, n_o$ )           ▷  $n_i$  is # inputs,  $n_o$  is #outputs
2:   for each  $0 \leq i \leq n_i$  and each  $0 \leq j < n_o$  do
3:      $d[i, j] := 0$ ;  $w[i, j] :=$  a random value
4:   def output(in)               ▷ in is array with length  $n_i$ 
5:     for each  $j$  do  $out[j] := w[n_i, j] + \sum_i in[i] * w[i, j]$ 
6:     return out
7:   def Backprop(error)         ▷ error is array with length  $n_o$ 
8:     for each  $i, j$  do  $d[i, j] := d[i, j] + in[i] * error[j]$ 
9:     for each  $i$  do  $ierror[i] := \sum_j w[i, j] * error[j]$ 
10:    return ierror
11:   def update()                 ▷ update weights.  $\eta$  is learning rate.
12:     for each  $i, j$  do
13:        $w[i, j] := w[i, j] - \eta / batch\_size * d[i, j]$ 
14:        $d[i, j] := 0$ 
```

Problems for (stochastic) gradient descent

Error as a function of parameters x and y :



Want different step sizes for x and y .

With many parameters, treat each parameter independently.

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 - 1: **def** *update*() ▷ update all weights
 - 2: **for each** *i, j* **do**
 - 3: $v[i, j] := \alpha * v[i, j] - \eta / \text{batch_size} * d[i, j]$
 - 4: $w[i, j] := w[i, j] + v[i, j]$
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2:   for each  $i, j$  do
3:      $g := d[i, j] / \text{batch\_size}$ 
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 - 5: $s[i, j] := \beta_1 * s[i, j] + (1 - \beta_1) * g$
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 - 7: $w[i, j] := w[i, j] - \frac{\eta * s[i, j] / (1 - \beta_1^t)}{\sqrt{r[i, j] / (1 - \beta_2^t)} + \epsilon}$
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- What happens at first step (when t becomes 1)?

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- What happens if the weights in the hidden layers are all set to the same value?
- For the output units, non-bias weights can be set to zero and the bias weights to the mean for regression or inverse-sigmoid of the empirical probability for classification. (Why?)

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In this case you should simplify the model.
- Then carry out **hyperparameter tuning**.
- If the performance isn't adequate, try to collect more data!
- Data augmentation can be a way to get more data, e.g., adding noise, scaling, translating or rotating images. (What can go wrong?)

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- batch size
- $L1$ and $L2$ regularization parameters.

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