Optimization and Generalization

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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  The value of variable X_i goes from v_i to $v_i - \eta \frac{\partial h}{\partial X_i}$.
  η is the step size.
- 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.

Differentiation

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 $f(e) = f_n(f_{n-1}(\ldots f_2(f_1(x_e))))$, 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:

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

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.

Neural-network learner

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

repeat
    batch := random sample of *batch_size* examples
    for each example *e* in *batch* **do**
        for each input unit *i* **do** $values[i] := X_i(e)$
        for each *fun* in *functions* from lowest to highest **do**
            $values := fun.output(values)$
        for each output unit *j* **do**
$error[j] := \phi_o(values[j]) - Ys[j]$
        for each *fun* in *functions* from highest to lowest **do**
            $error := fun.Backprop(error)$
    for each *fun* in *functions* that contains weights **do**
        $fun.update()$
until termination

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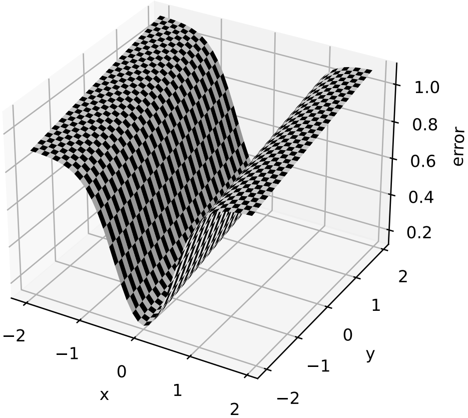
Dense linear function

```
class Dense(n_i, n_o)                         ▷ n_i is # inputs, n_o is #outputs
    for each 0 ≤ i ≤ n_i and each 0 ≤ j < n_o do
        d[i, j] := 0; w[i, j] := a random value
    def output(in)                            ▷ in is array with length n_i
        for each j do out[j] := w[n_i, j] + ∑_i in[i] ∗ w[i, j]
        return out
    def Backprop(error)                       ▷ error is array with length n_o
        for each i, j do d[i, j] := d[i, j] + in[i] ∗ error[j]
        for each i do ierror[i] := ∑_j w[i, j] ∗ error[j]
        return ierror
    def update()                              ▷ update weights. η is learning rate.
        for each i, j do
            w[i, j] := w[i, j] − η/batch_size ∗ d[i, j]
            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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def update()                                        ▷ update all weights
    for each i, j do
        v[i,j] := α ∗ v[i,j] − η/batch_size ∗ d[i,j]
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5: $w[i,j] := w[i,j] - \frac{\eta * g}{\sqrt{r[i,j] + \epsilon}}$
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    $t := t + 1$ ▷ t is initially 0
    for each i, j **do**
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        $r[i,j] := \beta_2 * r[i,j] + (1 - \beta_2) * g^2$
        $w[i,j] := w[i,j] - \dfrac{\eta * s[i,j]/(1 - \beta_1^t)}{\sqrt{r[i,j]/(1 - \beta_2^t)} + \epsilon}$
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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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- 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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