CSC321 Lecture 4: Learning a Classifier

Roger Grosse

Overview

- Last time: binary classification, perceptron algorithm
- Limitations of the perceptron
  - no guarantees if data aren't linearly separable
  - how to generalize to multiple classes?
  - linear model — no obvious generalization to multilayer neural networks
- This lecture: apply the strategy we used for linear regression
  - define a model and a cost function
  - optimize it using gradient descent

Overview

Design choices so far

- **Task:** regression, binary classification, multiway classification
- **Model/Architecture:** linear, log-linear
- **Loss function:** squared error, 0–1 loss, cross-entropy, hinge loss
- **Optimization algorithm:** direct solution, gradient descent, perceptron

Overview

- **Recall: binary linear classifiers.** Targets $t \in \{0, 1\}$

$$z = \mathbf{w}^T \mathbf{x} + b$$
$$y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

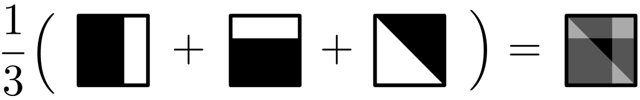
- Goal from last lecture: classify all training examples correctly
  - But what if we can't, or don't want to?
- Seemingly obvious loss function: 0-1 loss

$$\mathcal{L}_{0-1}(y, t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases}$$
$$= \mathbb{1}_{y \neq t}.$$

Attempt 1: 0-1 loss

- As always, the cost $\mathcal{E}$ is the average loss over training examples; for 0-1 loss, this is the error rate:

$$\mathcal{E} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{y^{(i)} \neq t^{(i)}}$$



middle region very good
since make no errors

Attempt 1: 0-1 loss

- Problem: how to optimize? cannot take derivative...
- Chain rule:

$$\frac{\partial \mathcal{L}_{0-1}}{\partial w_j} = \frac{\partial \mathcal{L}_{0-1}}{\partial z} \frac{\partial z}{\partial w_j}$$

Attempt 1: 0-1 loss

- Problem: how to optimize?
- Chain rule:

$$\frac{\partial \mathcal{L}_{0-1}}{\partial w_j} = \frac{\partial \mathcal{L}_{0-1}}{\partial z} \frac{\partial z}{\partial w_j}$$

- But $\partial \mathcal{L}_{0-1} / \partial z$ is zero everywhere it's defined!
  - $\partial \mathcal{L}_{0-1} / \partial w_j = 0$ means that changing the weights by a very small amount probably has no effect on the loss.
  - The gradient descent update is a no-op.

Attempt 2: Linear Regression

- Sometimes we can replace the loss function we care about with one which is easier to optimize. This is known as a surrogate loss function.
- We already know how to fit a linear regression model. Can we use this instead?

$$y = \mathbf{w}^\top \mathbf{x} + b$$

$$\mathcal{L}_{\mathrm{SE}}(y, t) = \frac{1}{2}(y - t)^2$$

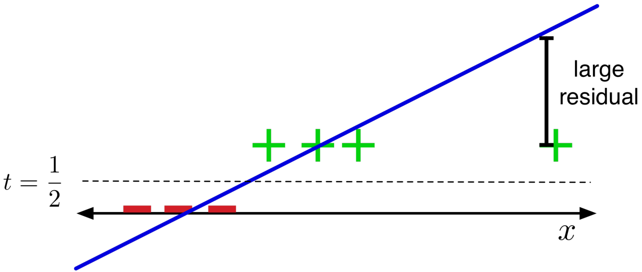
- Doesn't matter that the targets are actually binary.
- Threshold predictions at $y = 1/2$.

minimize scalar targets

Attempt 2: Linear Regression

The problem:

penalize a correct prediction
with large residuals if has larger leverage



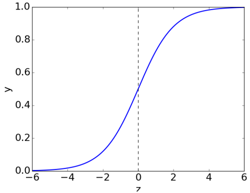
- The loss function hates when you make correct predictions with high confidence!
- If $t = 1$, it's more unhappy about $y = 10$ than $y = 0$.

Attempt 3: Logistic Activation Function

- There's obviously no reason to predict values outside [0, 1]. Let's squash y into this interval.

- The logistic function is a kind of sigmoidal, or S-shaped, function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



- A linear model with a logistic nonlinearity is known as log-linear:

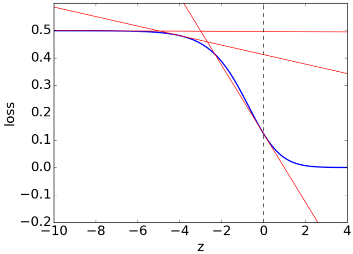
$$z = \mathbf{w}^\top \mathbf{x} + b$$
$$y = \sigma(z)$$
$$\mathcal{L}_{\mathrm{SE}}(y, t) = \frac{1}{2}(y - t)^2.$$

- Used in this way, σ is called an activation function, and z is called the logit.

Attempt 3: Logistic Activation Function

The problem:
(plot of $\mathcal{L}_{\mathrm{SE}}$ as a function of z)

dL/dz is slope on the curve



$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

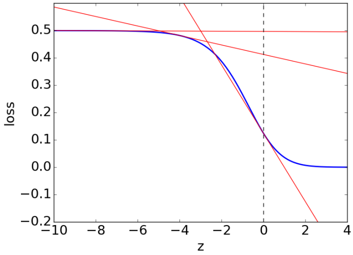
$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{L}}{\partial w_j}$$

problem: if really wrong, z very negative
we have close to 0 update to w

Attempt 3: Logistic Activation Function

The problem:

(plot of $\mathcal{L}_{\mathrm{SE}}$ as a function of z)



$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{L}}{\partial w_j}$$

- In gradient descent, a small gradient (in magnitude) implies a small step.
- If the prediction is really wrong, shouldn't you take a large step?

Logistic Regression

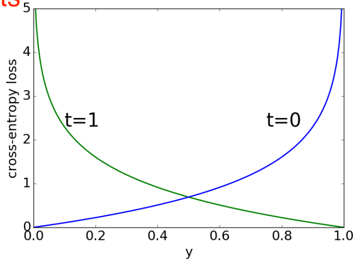
- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$.
- The pundits who were 99% confident Clinton would win were much more wrong than the ones who were only 90% confident.

Logistic Regression

- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$.
- The pundits who were 99% confident Clinton would win were much more wrong than the ones who were only 90% confident.
- Cross-entropy loss captures this intuition:

penalize predictions that are far from targets
i..e larger partial derivatives

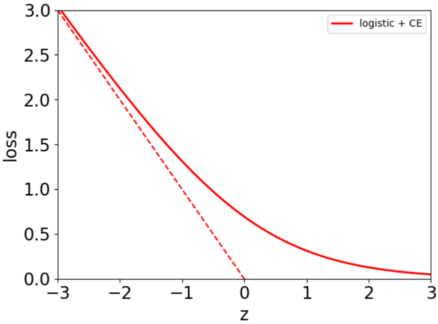
$$\mathcal{L}_{\mathrm{CE}}(y, t) = \begin{cases} -\log y & \text{if } t = 1 \\ -\log(1 - y) & \text{if } t = 0 \end{cases}$$
$$= -t \log y - (1 - t) \log(1 - y)$$



Logistic Regression

Logistic Regression:

$$
\begin{aligned}
z &= \mathbf{w}^\top \mathbf{x} + b \\
y &= \sigma(z) \\
&= \frac{1}{1 + e^{-z}} \\
\mathcal{L}_{\mathrm{CE}} &= -t \log y - (1 - t) \log(1 - y)
\end{aligned}
$$



[[gradient derivation in the notes]]

- Problem: what if $t = 1$ but you're really confident it's a negative example ($z \ll 0$)?
- If y is small enough, it may be numerically zero. This can cause very subtle and hard-to-find bugs.

$$y = \sigma(z) \qquad \Rightarrow y \approx 0$$

$$\mathcal{L}_{\mathrm{CE}} = -t \log y - (1-t)\log(1-y) \qquad \Rightarrow \text{ computes } \log 0$$

0 * infty

infinite loss

rounding errors -> zero

Logistic Regression

- Problem: what if $t = 1$ but you're really confident it's a negative example ($z \ll 0$)?
- If y is small enough, it may be numerically zero. This can cause very subtle and hard-to-find bugs.

$$
\begin{aligned}
y &= \sigma(z) & \Rightarrow\ & y \approx 0 \\
\mathcal{L}_{\text{CE}} &= -t \log y - (1-t)\log(1-y) & \Rightarrow\ & \text{computes } \log 0
\end{aligned}
$$

kind of breaks abstraction

- Instead, we combine the activation function and the loss into a single logistic-cross-entropy function.

$$
\mathcal{L}_{\text{LCE}}(z, t) = \mathcal{L}_{\text{CE}}(\sigma(z), t) = t \log(1 + e^{-z}) + (1-t)\log(1 + e^{z})
$$

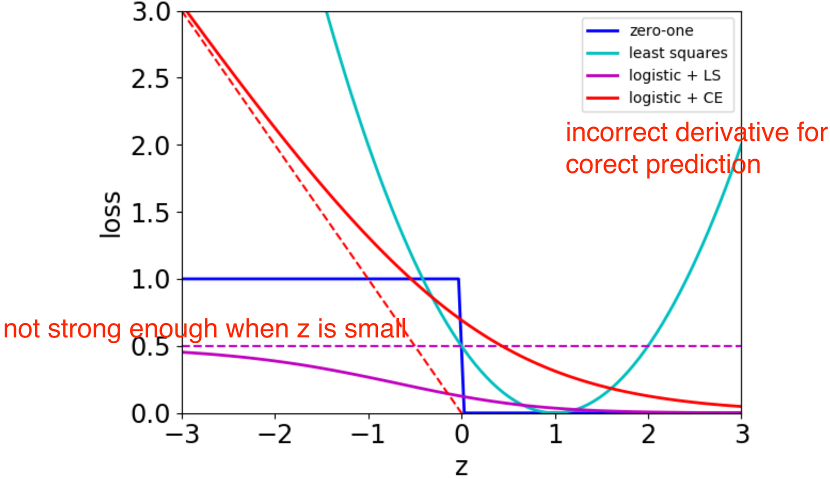
- Numerically stable computation:

```
E = t * np.logaddexp(0, -z) + (1-t) * np.logaddexp(0, z)
```

e^0 + e^{-z}

Logistic Regression

Comparison of loss functions:



Logistic Regression

Comparison of gradient descent updates:

- Linear regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)}$$

- Logistic regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)}$$

Logistic Regression

Comparison of gradient descent updates:

- Linear regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, \mathbf{x}^{(i)}$$

- Logistic regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, \mathbf{x}^{(i)}$$

- Not a coincidence! These are both examples of matching loss functions, but that's beyond the scope of this course.

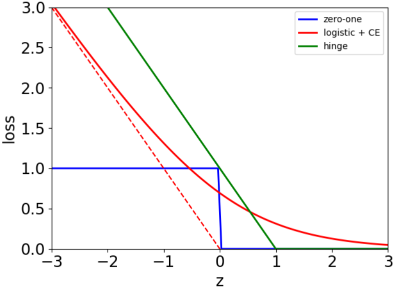
Hinge Loss

- Another loss function you might encounter is hinge loss. Here, we take $t \in \{-1, 1\}$ rather than $\{0, 1\}$.

$$\mathcal{L}_{\mathrm{H}}(y, t) = \max(0, 1 - ty)$$

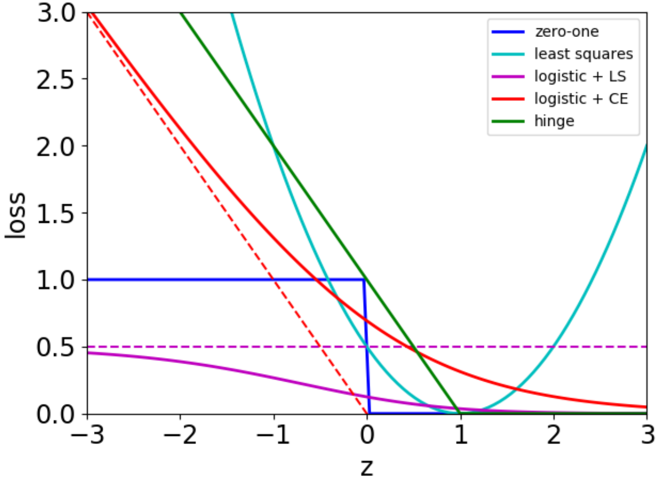
- This is an upper bound on 0-1 loss (a useful property for a surrogate loss function).
- A linear model with hinge loss is called a support vector machine. You already know enough to derive the gradient descent update rules!
- Very different motivations from logistic regression, but similar behavior in practice.

similar to logistic + CE, interchangeable



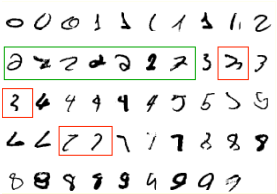
Logistic Regression

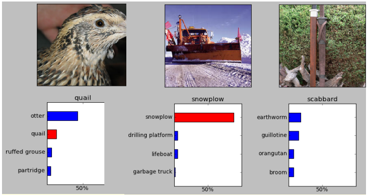
Comparison of loss functions:



Multiclass Classification

- What about classification tasks with more than two categories?





Multiclass Classification

- Targets form a discrete set $\{1, \ldots, K\}$.
- It's often more convenient to represent them as one-hot vectors, or a one-of-K encoding:

$$\mathbf{t} = \underbrace{(0, \ldots, 0, 1, 0, \ldots, 0)}_{\text{entry } k \text{ is } 1}$$

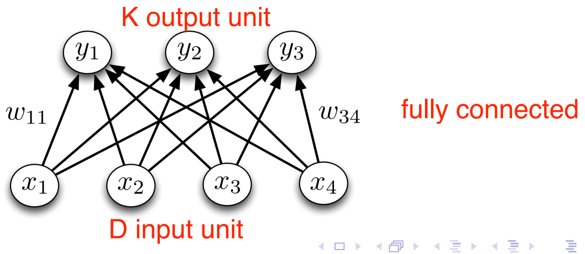
Multiclass Classification

- Now there are D input dimensions and K output dimensions, so we need $K \times D$ weights, which we arrange as a weight matrix $\mathbf{W}$.
- Also, we have a K-dimensional vector $\mathbf{b}$ of biases.
- Linear predictions:

$$z_k = \sum_j w_{kj} x_j + b_k$$

- Vectorized:

$$\mathbf{z} = \mathbf{W}\mathbf{x} + \mathbf{b}$$



Multiclass Classification

- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \mathrm{softmax}(z_1, \ldots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- The inputs z_k are called the logits.
- Properties:
  - Outputs are positive and sum to 1 (so they can be interpreted as probabilities)
  - If one of the z_k's is much larger than the others, $\mathrm{softmax}(\mathbf{z})$ is approximately the argmax. (So really it's more like "soft-argmax".)
  - **Exercise:** how does the case of $K = 2$ relate to the logistic function?
- Note: sometimes $\sigma(\mathbf{z})$ is used to denote the softmax function; in this class, it will denote the logistic function applied elementwise.

Multiclass Classification

- If a model outputs a vector of class probabilities, we can use cross-entropy as the loss function:

$$\begin{aligned}\mathcal{L}_{\mathrm{CE}}(\mathbf{y}, \mathbf{t}) &= -\sum_{k=1}^{K} t_k \log y_k \\ &= -\mathbf{t}^\top (\log \mathbf{y}),\end{aligned}$$

  where the log is applied elementwise.
- Just like with logistic regression, we typically combine the softmax and cross-entropy into a **softmax-cross-entropy** function.

Multiclass Classification

- Multiclass logistic regression:

$$
\begin{aligned}
\mathbf{z} &= \mathbf{W}\mathbf{x} + \mathbf{b} \\
\mathbf{y} &= \mathrm{softmax}(\mathbf{z}) \\
\mathcal{L}_{\mathrm{CE}} &= -\mathbf{t}^\top (\log \mathbf{y})
\end{aligned}
$$

- **Tutorial:** deriving the gradient descent updates

$$
\frac{\partial \mathcal{L}_{\mathrm{CE}}}{\partial \mathbf{z}} = \mathbf{y} - \mathbf{t}
$$

Convex Functions

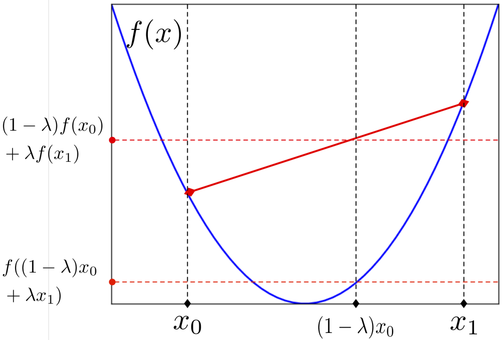
- Recall: a set $\mathcal{S}$ is convex if for any $\mathbf{x}_0, \mathbf{x}_1 \in \mathcal{S}$,

$$(1-\lambda)\mathbf{x}_0 + \lambda \mathbf{x}_1 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$

- A function f is convex if for any $\mathbf{x}_0, \mathbf{x}_1$ in the domain of f,

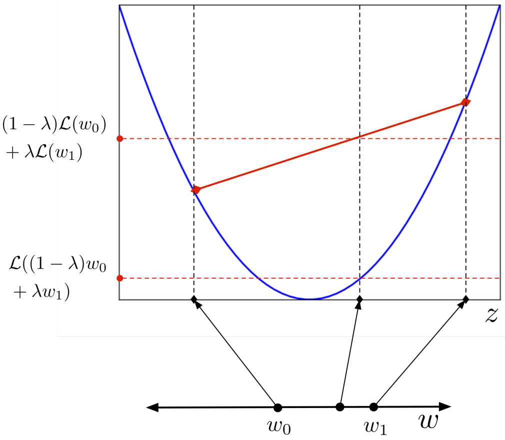
$$f((1-\lambda)\mathbf{x}_0 + \lambda \mathbf{x}_1) \leq (1-\lambda) f(\mathbf{x}_0) + \lambda f(\mathbf{x}_1)$$

- Equivalently, the set of points lying above the graph of f is convex.
- Intuitively: the function is bowl-shaped.

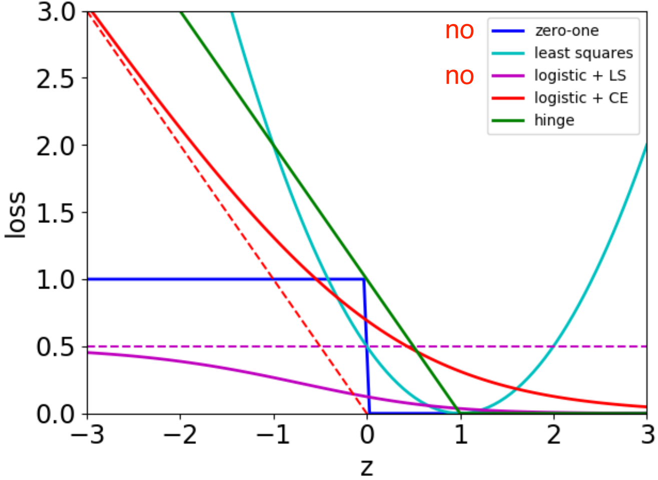


Convex Functions

- We just saw that the least-squares loss function $\frac{1}{2}(y - t)^2$ is convex as a function of y
- For a linear model, $z = \mathbf{w}^\top \mathbf{x} + b$ is a linear function of $\mathbf{w}$ and b. If the loss function is convex as a function of z, then it is convex as a function of $\mathbf{w}$ and b.



Which loss functions are convex?



Convex Functions

Why we care about convexity

- All critical points are minima
- Gradient descent finds the optimal solution (more on this in a later lecture)

Gradient Checking

- We've derived a lot of gradients so far. How do we know if they're correct?
- Recall the definition of the partial derivative:

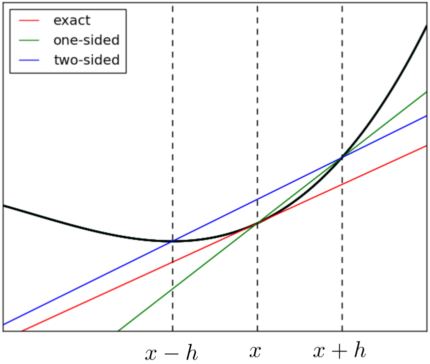
$$\frac{\partial}{\partial x_i} f(x_1, \ldots, x_N) = \lim_{h \to 0} \frac{f(x_1, \ldots, x_i + h, \ldots, x_N) - f(x_1, \ldots, x_i, \ldots, x_N)}{h}$$

- Check your derivatives numerically by plugging in a small value of h, e.g. 10^{-10}. This is known as finite differences.

Gradient Checking

- Even better: the two-sided definition

$$\frac{\partial}{\partial x_i} f(x_1, \ldots, x_N) = \lim_{h \to 0} \frac{f(x_1, \ldots, x_i + h, \ldots, x_N) - f(x_1, \ldots, x_i - h, \ldots, x_N)}{2h}$$



Gradient Checking

- Run gradient checks on small, randomly chosen inputs
- Use double precision floats (not the default for most deep learning frameworks!)
- Compute the relative error:

a,b are closed form solution for derivative and finite different approximation

$$\frac{|a - b|}{|a| + |b|}$$

- The relative error should be very small, e.g. 10^{-6}

Gradient Checking

- Gradient checking is really important!
- Learning algorithms often appear to work even if the math is wrong.
- **But:**
  - They might work much better if the derivatives are correct.
  - Wrong derivatives might lead you on a wild goose chase.
- If you implement derivatives by hand, gradient checking is the single most important thing you need to do to get your algorithm to work well.