TU-Delft Deep Learning course 2018-2019

02.MLrefresh

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Several slides credit to Roger Grosse

Questions?

Last time:

- Feed forward networks
- Stochastic gradient descent
- XOR

After this lecture you can:

- Understand maximum likelihood
- Explain the relation between a loss and gradient descent
- Understand binary classification with logistic regression
- Understand multiclass logistic regression

Book chapters: 3.10, 3.13, 5.5, 5.7.1, 6.2

Maximum likelihood estimation

Book: Chapter 5.5

- Training set of m samples $\mathbb{X} = \{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$
- Drawn i.i.d. from the true but unknown distribution $p_{\text{data}}(x)$
- Our model: Parametric family of probability distributions $p_{\text{model}}(x; \theta)$
- Maximum likelihood is $\theta_{ML} = \arg\max_\theta p_{\text{model}}(\mathbb{X}; \theta)$
- Rewrite in terms of data samples: $\arg\max_\theta \prod_{i=1}^m p_{\text{model}}(x^{(i)}; \theta)$
- Q: What assumption allowed this? A: i.i.d.
- Q: What is the problem with multiplying small values? A: goes to 0.
- Log: same maximum, turns multiplications to sums: $\arg\max_\theta \sum_{i=1}^m \log p_{\text{model}}(x^{(i)}; \theta)$
- Write as expectation wrt empirical distribution $\hat{p}_{\text{data}}$ as $\arg\max_\theta \mathbb{E}_{x\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(x; \theta)$,
- Q: Why is this the same? A: Dividing by m does not change the maximum

Minimize the dissimilarity of distributions

Book: 5.5, 3.13

- Max likelihood: $\arg\max_\theta \mathbb{E}_{x\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(x;\theta)$
- One interpretation: Minimize dissimilarity between $\hat{p}_{\text{data}}$ and p_{model}
- Measure dissimilarity by the KL divergence

  $D(p_{\text{data}}||p_{\text{model}}) = \sum_{i=1}^{m} \hat{p}_{\text{data}}(x^{(i)}) \log\left(\frac{p_{\text{data}}(x^{(i)})}{p_{\text{model}}(x^{(i)})}\right)$
- Q: rewrite in terms of data samples (expectation) and using logs?
- A: $\mathbb{E}_{x\sim\hat{p}_{\text{data}}}\left[\log p_{\text{data}}(x) - \log p_{\text{model}}(x)\right]$
- Left/data term $(\log p_{\text{data}}(x))$ does not depend on the model: Remove.
- So minimize $\mathbb{E}_{x\sim\hat{p}_{\text{data}}}[-\log p_{\text{model}}(x)]$
- Q: Relate $\arg\min_\theta -\mathbb{E}_{x\sim\hat{p}_{\text{data}}}[\log p_{\text{model}}(x)]$ to max likelihood? A: Same.

Cross-entropy

Book: 3.13

The literature optimizes “cross-entropy”.

- KL related to cross-entropy between two distributions $H(p_{\text{data}}, p_{\text{model}}) = H(p_{\text{data}}) + D(p_{\text{data}}||p_{\text{model}})$, where H is entropy.
- Q: What is the effect of $H(p_{\text{data}})$ on p_{model}?
- A: The model does not depend on $H(p_{\text{data}})$, so can be omitted.
- The term cross-entropy is generic, not just for classification (Bernoulli or softmax distributions).
- Eg: mean squared error is the cross-entropy between empirical distribution and a Gaussian.
- Minimize KL divergence $\Leftrightarrow$ minimize negative log likelihood $\Leftrightarrow$ minimize cross-entropy $\Leftrightarrow$ maximize maximum likelihood.

Conditional log-likelihood and output units

Book: 5.5.1 and 6.2.2

Often interested in classification problems

- Conditional log-likelihood: Predict labels Y given data X: $P(Y|X;\theta)$
- $\theta_{ML} = \arg\max_\theta P(Y|X;\theta)$
- Assume i.i.d.: $\arg\max_\theta \sum_{i=1}^{m} \log P(y^{(i)}|x^{(i)};\theta)$

What to optimize in a deep net:

- Usually: cross-entropy between data distribution and model distribution
- Output units determine the form of the cross-entropy function

Binary classification

Book: 3.10 and 6.2.2

Bernoulli distribution on $P(Y = 1|X)$, single number between $[0, 1]$

- Q: Why is a single number enough for two classes?
- A: $P(Y = 0|X) = 1 - P(Y = 1|X)$

Lets try linear unit $P(Y = 1|X) = \max\left\{0, \min\left\{1, w^\top h + b\right\}\right\} = y$ for features h

- Q: No loss defined, but what happens to the gradients outside interval $[0, 1]$?
- A: No more gradients: Cannot be optimized by gradient descent

Making optimization easier

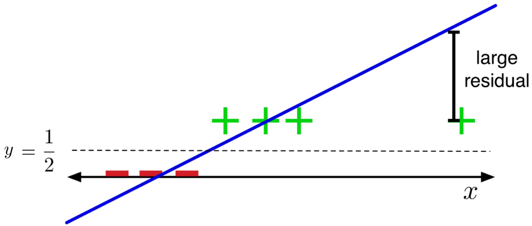
Book: 6.2.2.2

The min/max prevent gradient flow $P(Y = 1|X) = \max\left\{0, \min\left\{1, w^\top h + b\right\}\right\}$

- Q: How could you make them flow again?
- A: One answer: remove min/max
- Q: Continue output; how to binarize to two classes?
- A: Threshold predictions y at $y = \frac{1}{2}$

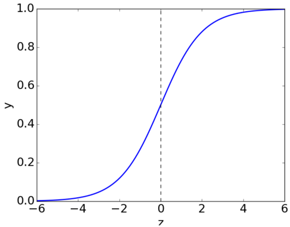
loss wants to be exact

Lets use a square loss, $P(Y=1|X) = \frac{1}{2}((w^\top h + b) - t)^2$, t=true label



- Q: What is the problem here?
- A: Large losses for predictions with high confidence.
- If $t = 1$, loss is higher for $y = 10$ then for $y = 0$.

- Q: Other way to limit the output to $[0, 1]$?
- A: Squash it between 0 and 1.
- The logistic function is sigmoidal (S-shaped)



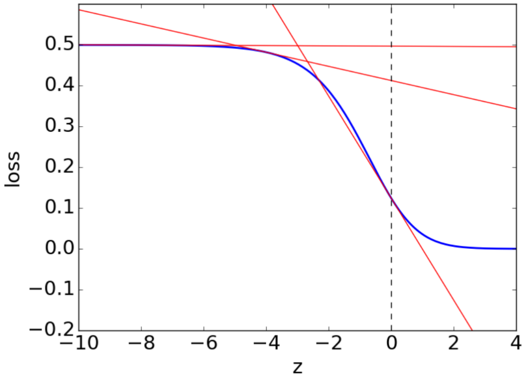
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

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

$$z = w^\top x + b$$
$$y = \sigma(z)$$
$$\mathcal{L}_{\mathsf{SE}} = \frac{1}{2}(y - t)^2 \qquad \text{(SE: Squared Error)}$$

Where σ is the activation function and z is called the logit.

Lets look at the derivatives



Derivatives of squared error loss with logistic nonlinearity for a positive sample.

- Q: What is the problem here?
- A: Gradient descent: small gradient is a small step.
- Should take large step when the prediction is really wrong

Logistic regression

Replace squared loss with Bernoulli cross-entropy loss

- Bernoulli: y if $t = 1$ and $1 - y$ if $t = 0$, t=true label

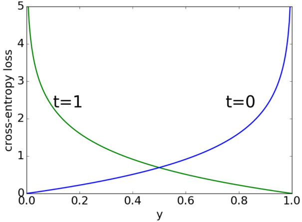
Q: What is the Bernoulli cross entropy loss?

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

Same as: $-t \log y - (1 - t) \log(1 - y)$

Q: Why is this the same?

Q: Draw graphs for $t = 1$ and $t = 0$?



t=true label

Q: What is penalized?

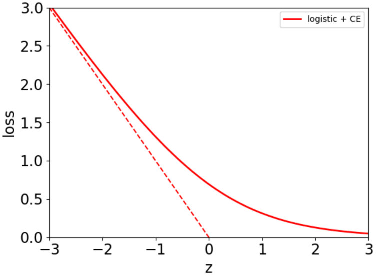
A: Penalizes small difference of really wrong predictions

Logistic regression

$$z = w^\top x + b$$

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

$$\mathcal{L}_{\text{CE}} = -t \log y - (1 - t) \log(1 - y)$$



Q: Explain the terms on the left

Q: What is shown on this graph?

A: The loss for $t = 1$

Q: What does it penalize?

A: Penalizes very wrong predictions

Multiclass classification

Book: 6.2.2.3

- Targets from a discrete set $\{1, \ldots, K\}$
- Convenient: "One-of-K", or "One-hot" encoding:

$$t = \underbrace{(0, \ldots, 0, 1, 0, \ldots, 0)}_{\text{Entry } k \text{ is set to 1}}$$

- Softmax: generalization of logistic function:

$$Y_k = \mathsf{softmax}(z_1, z_2, \ldots, z_K) = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- Vector of class probabilities, use cross-entropy as loss function

$$\mathcal{L}_{\mathsf{CE}}(y, t) = -\sum_{k=1}^{K} t_k \log y_k = -t^\top (\log y)$$

- Outputs positive and sum to 1. (Probabilistic interpretation)
- If one of the z_k is much larger, it approximates the arg max.

Questions?