Differentiable Relaxations and Reparameterisations

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What are differentiable relaxations and reparameterisations?

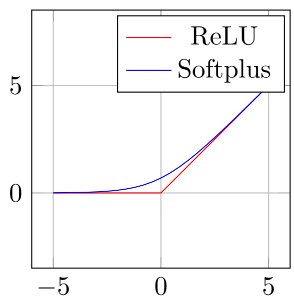
- We've seen that we can build arbitrary computational graphs from a variety of building blocks
- But, those blocks need to be differentiable to work in our optimisation framework
  - More specifically they need to be continuous and *differentiable almost everywhere*.
- That limits what we can do... Can we work around that?
  - Relaxations — make continuous (and potentially differentiable everywhere) approximations.
  - Reparameterisations — rewrite functions to factor out stochastic variables from the parameters.

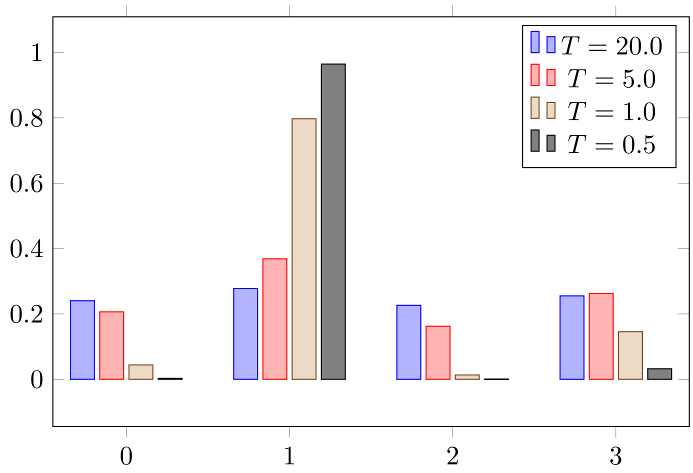
Aside: continuity and differentiable almost everywhere

- Consider the ReLU function $f(x) = max(0, x)$
  - ReLU is *continuous*
    - it does not have any abrupt changes in value
    - small changes in x result in small changes to $f(x)$ everywhere in the domain of x
  - ReLU is *differentiable almost everywhere*
    - No gradient at $x = 0$; only *left* and *right* gradients at that point
    - There are *subgradients* at $x = 0$; implementations usually just arbitrarily pick $f'(0) = 0$
- Functions that are differentiable almost everywhere or have subgradients tend to be compatible with gradient descent methods
  - We expect that the loss landscape is different for each batch & that we'll never actually reach a minima, and we only need to *mostly* take steps in the right direction.

Relaxing ReLU

- Softplus ($\text{softplus}(x) = \ln(1 + e^x)$) is a relaxation of ReLU that is *differentiable everywhere*.
- Its derivative is the Sigmoid function
- Not widely used; counter-intuitively, even though it neither saturates completely and is differentiable everywhere, empirically it has been shown that ReLU works better.





Interpretations of softmax

- Up until now we've really considered softmax as a generalisation of sigmoid (which represents a probability distribution over a binary variable) to many output categories.
  - softmax transforms a vector of logits into a probability distribution over categories.
- As you might guess from the name, softmax is a relaxation...
  - but not of the max function like the name would suggest!
  - softmax can be viewed as a continuous and differentiable relaxation of the arg max function with one-hot output encoding.
  - The arg max function is not continuous or differentiable; softmax provides an approximation:

$$
\begin{array}{rlllll}
\boldsymbol{x} = & [\; 1.1 & 4.0 & \text{-}0.1 & 2.3 &] \\
\arg\max(\boldsymbol{x}) = & [\; 0 & 1 & 0 & 0 &] \\
\mathrm{softmax}(\boldsymbol{x}) = & [\; 0.044 & 0.797 & 0.013 & 0.146 &]
\end{array}
$$

The Softmax function with temperature

Consider what happens if you were to divide the input logits to a softmax by a scalar temperature parameter T.

$$\mathrm{softmax}(\boldsymbol{x}/T)_i = \frac{e^{x_i/T}}{\sum_{j=1}^{K} e^{x_j/T}} \qquad \forall i = 1, 2, \ldots, K$$

$\arg\max$ — softmax **with temperature**

$$
\begin{array}{rlllll}
\boldsymbol{x} = & [\; 1.1 & 4.0 & \text{-}0.1 & 2.3 &] \\
\mathrm{softmax}(\boldsymbol{x}/1.0) = & [\; 0.044 & 0.797 & 0.013 & 0.146 &] \\
\mathrm{softmax}(\boldsymbol{x}/0.8) = & [\; 0.023 & 0.868 & 0.005 & 0.104 &] \\
\mathrm{softmax}(\boldsymbol{x}/0.6) = & [\; 0.008 & 0.937 & 0.001 & 0.055 &] \\
\mathrm{softmax}(\boldsymbol{x}/0.4) = & [\; 6.997\text{e-}04 & 9.852\text{e-}01 & 3.484\text{e-}05 & 1.405\text{e-}02 &] \\
\mathrm{softmax}(\boldsymbol{x}/0.2) = & [\; 5.042\text{e-}07 & 9.998\text{e-}01 & 1.250\text{e-}09 & 2.034\text{e-}04 &]
\end{array}
$$

$\arg\max$ — **scalar approximation**

- What if you want to get a scalar approximation to the index of the arg max rather than a probability distribution approximating the one-hot form?
  - Caveat: we are not actually going get a guaranteed integer representation as that would be non-differentiable; we'll have to live with a float that is an approximation[1].

[1] for now — we'll address this in a few slides time!

- First, consider how to convert a one-hot vector to index representation in a differentiable manner: $[0, 0, 1, 0] \to 2$
  - Just dot product with a vector of indices: $[0, 1, 2, 3]$
- The same process can be applied to the softmax distribution
  - As temperature $T \to 0$, $\text{softmax}(\boldsymbol{x}/T) \cdot [0, 1, \ldots, N] \to \arg\max(\boldsymbol{x})$ for $\boldsymbol{x} \in \mathbb{R}^N$.

$\arg\max$ — **scalar approximation**

$$
\begin{aligned}
\boldsymbol{x} &= [\ 1.1 \quad 4.0 \quad -0.1 \quad 2.3\ ]^\top \\
\boldsymbol{i} &= [\ 0.0 \quad 1.0 \quad 2.0 \quad 3.0\ ]^\top \\
\text{softmax}(\boldsymbol{x}/1.0)^\top \boldsymbol{i} &= 1.2606 \\
\text{softmax}(\boldsymbol{x}/0.8)^\top \boldsymbol{i} &= 1.1894 \\
\text{softmax}(\boldsymbol{x}/0.6)^\top \boldsymbol{i} &= 1.1037 \\
\text{softmax}(\boldsymbol{x}/0.4)^\top \boldsymbol{i} &= 1.0274 \\
\text{softmax}(\boldsymbol{x}/0.2)^\top \boldsymbol{i} &= 1.0004
\end{aligned}
$$

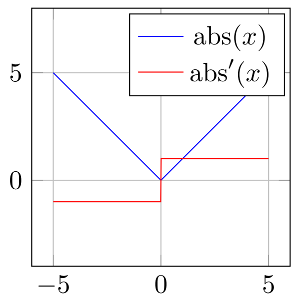
max

- A similar trick applies to finding the maximum value of a vector:
  - Use $\text{softmax}(\boldsymbol{x})$ as an approximate one-hot $\arg\max$, and dot product with the vector $\boldsymbol{x}$.
  - As temperature $T \to 0$, $\text{softmax}(\boldsymbol{x}/T)^\top \boldsymbol{x} \to \max(\boldsymbol{x})$.

$$
\begin{aligned}
\boldsymbol{x} &= [\ 1.1 \quad 4.0 \quad -0.1 \quad 2.3\ ]^\top \\
\text{softmax}(\boldsymbol{x}/1.0)^\top \boldsymbol{x} &= 3.571 \\
\text{softmax}(\boldsymbol{x}/0.8)^\top \boldsymbol{x} &= 3.736 \\
\text{softmax}(\boldsymbol{x}/0.6)^\top \boldsymbol{x} &= 3.881 \\
\text{softmax}(\boldsymbol{x}/0.4)^\top \boldsymbol{x} &= 3.974 \\
\text{softmax}(\boldsymbol{x}/0.2)^\top \boldsymbol{x} &= 3.999
\end{aligned}
$$

L1 norm

- L1 norm is the sum of absolute values of a vector
- We've seen that an L1 norm regulariser can induce sparsity in a model
- abs is continuous and differentiable almost everywhere, but...
- unlike ReLU, the gradients left and right of the discontinuity point in equal and opposite directions
  - This can cause oscillations that prevent or hamper learning

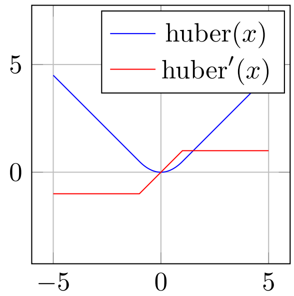


Relaxing the L1 norm

- Huber loss (aka Smooth L1 loss) relaxes L1 by mixing it with L2 near the origin:

$$z_i = \begin{cases} 0.5(x_i - y_i)^2, & \text{if } |x_i - y_i| < 1 \\ |x_i - y_i| - 0.5, & \text{otherwise} \end{cases}$$

- In both cases gradients reduce in magnitude and switch direction smoothly which can lead to much less oscillation.



Backpropagation through random operations

- Up until now all the models we've considered have performed deterministic transformations of input variables $\boldsymbol{x}$.
- What if we want to build a model that performs a stochastic transformation of $\boldsymbol{x}$?
- A simple way to do this is to augment the input $\boldsymbol{x}$ with a random vector $\boldsymbol{z}$ sampled from some distribution
  - The network would learn a function $f(\boldsymbol{x}, \boldsymbol{z})$ that is internally deterministic, but appears stochastic to an observer that does not have access to $\boldsymbol{z}$.
  - provided that f is continuous and differentiable (almost everywhere) we can perform gradient based optimisation as usual.

Differentiable Sampling

Consider

$$y \sim \mathcal{N}(\mu, \sigma^2)$$

How can we take derivatives of y with respect to μ and σ^2?

Differentiable Sampling

If we rewrite

$$y = \mu + \sigma z \text{ where } z = \mathcal{N}(0, 1)$$

Then it is clear that y is a function of a deterministic operation with variables μ and σ with an (extra) input z.

- Crucially the extra input is an r.v. whose distribution is not a function of any variables whose derivatives we wish to calculate.
- The derivatives $dy/d\mu$ and $dy/d\sigma$ tell us how an infinitesimal change in μ or σ would change y if we could repeat the sampling operation with the *same* value of z

The reparameterisation trick

- The 'trick' of factoring out the source of randomness into an extra input z is often called the **reparameterisation trick**.
- It doesn't just apply to the Gaussian distribution!
  - More generally we can express any probability distribution $p(\mathrm{y}; \boldsymbol{\theta})$ or $p(\mathrm{y}|\boldsymbol{x}; \boldsymbol{\theta})$ as $p(\mathrm{y}; \boldsymbol{\omega})$ where $\boldsymbol{\omega}$ contains the parameters $\boldsymbol{\theta}$ and if applicable inputs $\boldsymbol{x}$.

  - A sample $\boldsymbol{y} \sim p(\mathrm{y}; \boldsymbol{\omega})$ can be rewritten as $\boldsymbol{y} = f(\boldsymbol{z}, \boldsymbol{\omega})$ where $\boldsymbol{z}$ is a source of randomness.
  - We can thus compute derivatives $\partial \boldsymbol{y} / \partial \boldsymbol{\omega}$ and use gradient based optimisation as long as
    * f is continuous and differentiable almost everywhere
    * $\boldsymbol{\omega}$ is not a function of $\boldsymbol{z}$
    * and $\boldsymbol{z}$ is not a function of $\boldsymbol{\omega}$

Backpropagation through discrete stochastic operations

- Consider a stochastic model $\boldsymbol{y} = f(\boldsymbol{z}, \boldsymbol{\omega})$ where the outputs are **discrete**.
  - This implies f must be a step function.
  - Derivatives of a step function at the step are undefined.
  - Derivatives are zero almost everywhere.
  - If we have a loss $\mathcal{L}(\boldsymbol{y})$ the gradients don't give us any information on how to update the parameters $\boldsymbol{\theta}$ to minimise the loss
- Potential solutions:
  - Policy Gradient Methods (e.g. the REINFORCE algorithm)
  - A relaxation and another 'trick': Gumbel Softmax and the Straight-through operator

REINFORCE: REward Increment = nonnegative Factor × Offset Reinforcement × Characteristic Eligibility

- $\mathcal{L}(f(\boldsymbol{z}, \boldsymbol{\omega}))$ has useless derivatives
- But the expected loss $\mathbb{E}_{\boldsymbol{z} \sim p(\mathbf{z})} \mathcal{L}(f(\boldsymbol{z}, \boldsymbol{\omega}))$is often smooth and continuous.
  - This is not tractable with high dimensional $\boldsymbol{y} = f(\boldsymbol{z}, \boldsymbol{\omega})$.
  - But, it can be estimated without bias using an Monte Carlo average.
- REINFORCE is a family of algorithms that utilise this idea.

REINFORCE: REward Increment = nonnegative Factor × Offset Reinforcement × Characteristic Eligibility

The simplest form of REINFORCE is easy to derive by differentiating the expected loss:

$$\mathbb{E}_{\boldsymbol{z}}[\mathcal{L}(\boldsymbol{y})] = \sum_{\boldsymbol{y}} \mathcal{L}(\boldsymbol{y}) p(\boldsymbol{y}) \tag{1}$$

$$\frac{\partial \mathbb{E}[\mathcal{L}(\boldsymbol{y})]}{\partial \boldsymbol{\omega}} = \sum_{\boldsymbol{y}} \mathcal{L}(\boldsymbol{y}) \frac{\partial p(\boldsymbol{y})}{\partial \boldsymbol{\omega}} \tag{2}$$

$$= \sum_{\boldsymbol{y}} \mathcal{L}(\boldsymbol{y}) p(\boldsymbol{y}) \frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}} \tag{3}$$

$$\approx \frac{1}{m} \sum_{\boldsymbol{y}^{(i)} \sim p(\mathbf{y}), i=1}^{m} \mathcal{L}(\boldsymbol{y}^{(i)}) \frac{\partial \log p(\boldsymbol{y}^{(i)})}{\partial \boldsymbol{\omega}} \tag{4}$$

- This gives us an unbiased MC estimator of the gradient.
- Unfortunately this is a very high variance estimator, so it would require many samples of y to be drawn to obtain a good estimate
  - or equivalently, if only one sample were drawn, SGD would converge very slowly and **require** a small learning rate.

Sampling from a categorical distribution: Gumbel Softmax

The generation of a discrete token, t, from a vocabulary of K tokens is achieved by sampling a categorical distribution

$$t \sim \text{Cat}(p_1, \dots, p_K)\,;\, \sum_i p_i = 1.$$

Generating the probabilities $p_1, \dots, p_K$ directly from a neural network has potential numerical problems; it's much easier to generate logits, $x_1, \dots, x_K$. [0.5em] The gumbel-softmax reparameterisation allows us to sample directly using the logits:

$$t = \underset{i \in \{1, \cdots, K\}}{\text{argmax}}\ x_i + z_i$$

where $z_1, \dots z_K$ are i.i.d Gumbel(0,1) variates which can be computed from Uniform variates through $-\log(-\log(\mathcal{U}(0,1)))$.

Differentiable Sampling: Straight-Through Gumbel Softmax

Ok, but how does that help? argmax isn't differentiable! [0.5em] ...but we've already seen that we can relax $\arg\max$ using

$$\text{softargmax}(\boldsymbol{y}) = \sum_i \frac{e^{y_i/T}}{\sum_j e^{y_j/T}} i$$

where T is the temperature parameter.

Differentiable Sampling: Straight-Through Gumbel Softmax

But... this clearly gives us a result that will be non-integer; we cannot round or clip because it would be non-differentiable. [0.5em] The Straight-Through operator allows us to take the result of a true argmax that has the gradient of the softargmax:

$$\text{STargmax}(\boldsymbol{y}) = \text{softargmax}(\boldsymbol{y}) + \text{stopgradient}(\text{argmax}(\boldsymbol{y}) - \text{softargmax}(\boldsymbol{y}))$$

where stopgradient is defined such that $\text{stopgradient}(\boldsymbol{a}) = \boldsymbol{a}$ and $\nabla\, \text{stopgradient}(\boldsymbol{a}) = 0$.

Straight-Through Gumbel Softmax

Combine the gumbel softmax trick with the STargmax to give you discrete samples, with a usable gradient[2].

Summary

- Differentiable programming works with functions that are continuous and differentiable almost everywhere.
- Some non-continuous functions can be relaxed to make them more amenable to gradient based optimisation by making continuous approximations.
- Some continuous functions with discontinuous gradients can be relaxed to make optimisation more stable.
- Reparameterisations can allow us to differentiate through random operations such as sampling
- We can even make networks output/utilise discrete variables by combining relaxations and reparameterisations.

[2]The ST operator is biased but low variance; in practice it works very well and is better than the high-variance unbiased estimates you could get through REINFORCE.