

Differentiate Almost Everywhere

VLC = \iiint Vision
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Differentiable Relaxations and Reparameterisations

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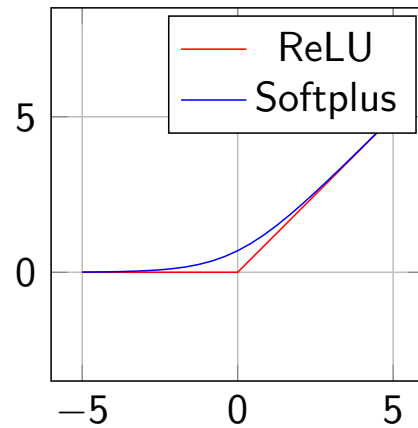
What are differentiable relaxations and reparameterisations?

- 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.

- 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

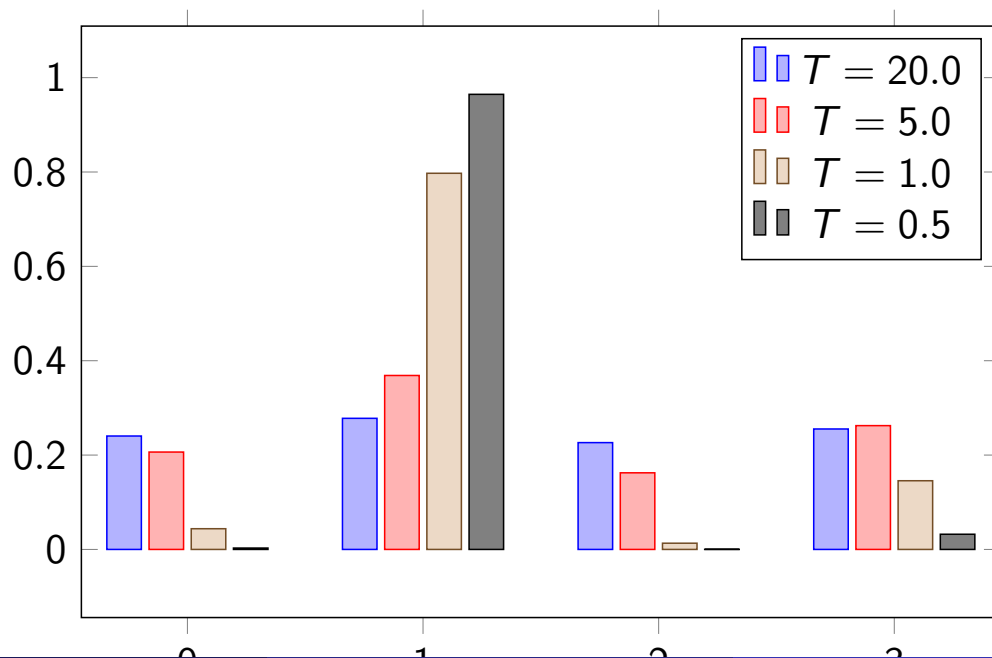
- Up until now we've really considered softmax as a generalisation of sigmoid (which represents a probability distribution over a binary variable) to many output categories.
 - softmax transforms a vector of logits into a probability distribution over categories.
- As you might guess from the name, softmax 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:

$$\begin{aligned} \mathbf{x} &= \begin{bmatrix} 1.1 & 4.0 & -0.1 & 2.3 \end{bmatrix} \\ \arg \max(\mathbf{x}) &= \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix} \\ \text{softmax}(\mathbf{x}) &= \begin{bmatrix} 0.044 & 0.797 & 0.013 & 0.146 \end{bmatrix} \end{aligned}$$

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 .

$$\text{softmax}(\mathbf{x}/T)_i = \frac{e^{x_i/T}}{\sum_{j=1}^K e^{x_j/T}} \quad \forall i = 1, 2, \dots, K$$



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Relaxation

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arg max — softmax with temperature

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

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Relaxation

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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 to get a guaranteed integer representation as that would be non-differentiable; we'll have to live with a float that is an approximation¹.
- First, consider how to convert a one-hot vector to index representation in a differentiable manner: $[0, 0, 1, 0] \rightarrow 2$
 - Just dot product with a vector of indices: $[0, 1, 2, 3]$
- The same process can be applied to the softmax distribution
 - As temperature $T \rightarrow 0$, $\text{softmax}(\mathbf{x}/T) \cdot [0, 1, \dots, N] \rightarrow \arg \max(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^N$.

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

arg max — scalar approximation

$$\mathbf{x} = [1.1 \quad 4.0 \quad -0.1 \quad 2.3]^\top$$

$$\mathbf{i} = [0.0 \quad 1.0 \quad 2.0 \quad 3.0]^\top$$

$$\text{softmax}(\mathbf{x}/1.0)^\top \mathbf{i} = 1.2606$$

$$\text{softmax}(\mathbf{x}/0.8)^\top \mathbf{i} = 1.1894$$

$$\text{softmax}(\mathbf{x}/0.6)^\top \mathbf{i} = 1.1037$$

$$\text{softmax}(\mathbf{x}/0.4)^\top \mathbf{i} = 1.0274$$

$$\text{softmax}(\mathbf{x}/0.2)^\top \mathbf{i} = 1.0004$$

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

$$\mathbf{x} = [1.1 \quad 4.0 \quad -0.1 \quad 2.3]^\top$$

$$\text{softmax}(\mathbf{x}/1.0)^\top \mathbf{x} = 3.571$$

$$\text{softmax}(\mathbf{x}/0.8)^\top \mathbf{x} = 3.736$$

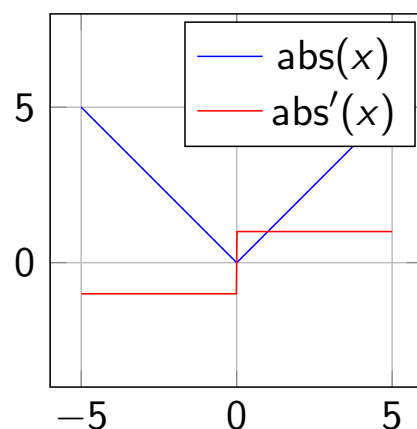
$$\text{softmax}(\mathbf{x}/0.6)^\top \mathbf{x} = 3.881$$

$$\text{softmax}(\mathbf{x}/0.4)^\top \mathbf{x} = 3.974$$

$$\text{softmax}(\mathbf{x}/0.2)^\top \mathbf{x} = 3.999$$

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

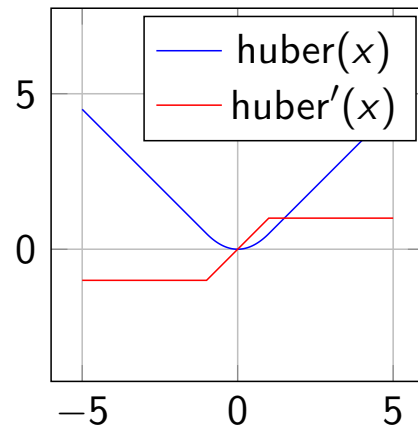


Relaxing the L1 norm

- 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 \mathbf{x} .
- What if we want to build a model that performs a stochastic transformation of \mathbf{x} ?
- A simple way to do this is to augment the input \mathbf{x} with a random vector \mathbf{z} sampled from some distribution
 - The network would learn a function $f(\mathbf{x}, \mathbf{z})$ that is internally deterministic, but appears stochastic to an observer that does not have access to \mathbf{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 \mathbf{z} is often called the **reparameterisation trick**.
- It doesn't just apply to the Gaussian distribution!
 - More generally we can express any probability distribution $p(\mathbf{y}; \boldsymbol{\theta})$ or $p(\mathbf{y}|\mathbf{x}; \boldsymbol{\theta})$ as $p(\mathbf{y}; \boldsymbol{\omega})$ where $\boldsymbol{\omega}$ contains the parameters $\boldsymbol{\theta}$ and if applicable inputs \mathbf{x} .
 - A sample $\mathbf{y} \sim p(\mathbf{y}; \boldsymbol{\omega})$ can be rewritten as $\mathbf{y} = f(\mathbf{z}, \boldsymbol{\omega})$ where \mathbf{z} is a source of randomness.
 - We can thus compute derivatives $\partial \mathbf{y} / \partial \boldsymbol{\omega}$ and use gradient based optimisation as long as
 - f is continuous and differentiable almost everywhere
 - $\boldsymbol{\omega}$ is not a function of \mathbf{z}
 - and \mathbf{z} is not a function of $\boldsymbol{\omega}$

Backpropagation through discrete stochastic operations

- Consider a stochastic model $\mathbf{y} = f(\mathbf{z}, \boldsymbol{\omega})$ 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 $\mathcal{L}(\mathbf{y})$ 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 \times Offset Reinforcement \times Characteristic Eligibility

- $\mathcal{L}(f(\mathbf{z}, \boldsymbol{\omega}))$ has useless derivatives
- But the expected loss $\mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathcal{L}(f(\mathbf{z}, \boldsymbol{\omega}))$ is often smooth and continuous.
 - This is not tractable with high dimensional $\mathbf{y} = f(\mathbf{z}, \boldsymbol{\omega})$.
 - 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 \times Offset Reinforcement \times Characteristic Eligibility

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

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

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

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

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

- 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 \mathbf{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 .

The gumbel-softmax reparameterisation allows us to sample directly using the logits:

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

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!

...but we've already seen that we can relax argmax using

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

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.

The Straight-Through operator allows us to take the result of a true argmax that has the gradient of the softargmax:

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

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

Straight-Through Gumbel Softmax

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

^aThe 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.

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.