# Linear models for regression and classification

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## 1 Supervised learning

Setup and examples

Loss functions

Building a loss function

# (Informal) definition of supervised learning

A (supervised) dataset is a set of $n$ examples:

$$\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \; . \tag{1}$$

Informally, given a 'new' pair $(x, y)$ not contained in $\mathcal{S}$, we want a function $f(\cdot)$ such that:

$$f(x) \approx y \, . \tag{2}$$

More generally, we can test the model on a separate dataset $\mathcal{T}$ never seen during training, i.e., $\mathcal{S} \bigcap \mathcal{T} = \emptyset$.

# Constraints on the dataset

We always assume implicitly that the elements in $\mathcal{S}$ and the elements in $\mathcal{T}$ are taken from *the same* i.i.d, *unknown* distribution $p(x, y)$.

- **Identically distributed**: the data-generating process is stable (e.g., in recognizing cats, the distribution of species do not change).
- **Independently distributed**: there is no bias in the data collection (e.g., we mostly collect siamese cats).

If the distribution between $\mathcal{S}$ and $\mathcal{T}$ varies, we talk about domain shift.

# Some motivating examples

1. **Spam identification**: $x_i$ is an email, and $y_i$ describes its probability of being spam.
2. **Robot navigation**: $x_i$ is a sensory representation of the environment, and $y_i$ is a motor command.
3. **Text translation**: $x_i$ is a text and $y_i$ its corresponding translation.
4. **Product recommendation**: $x_i$ is a user, and $y_i$ its affinity w.r.t. a certain catalogue of products.

**Note**: ensuring the i.i.d. property sometimes is far from trivial!

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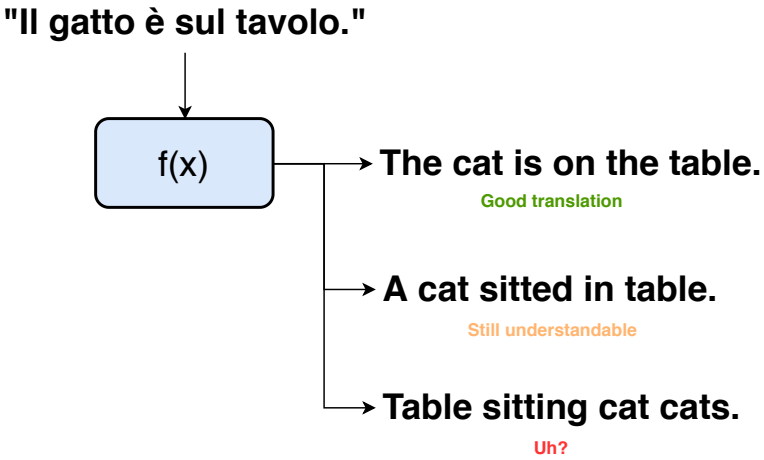
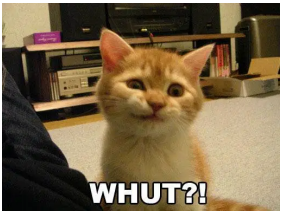
# What is a good approximation?



# Introducing loss functions

Given a point $x$, a desired value $y$, and a prediction $\hat{y} = f(x)$, we formalize its quality with a loss function $l(y, \hat{y})$, such that:

1. Low value of loss: good approximation;
2. High value of loss: poor approximation.

In this way, learning becomes a problem of minimizing a certain loss quantity that we designed. Importantly, the loss function should be a scalar, vary gradually, and (as we will see) be differentiable.

# Expected risk and empirical risk

The expected loss (risk) of a function $f$ is:

$$f^*(x) = \arg\min \left\{ \mathbb{E}_{p(x,y)} \left[ l(y, f(x)) \right] \right\} . \tag{3}$$

The expected risk is uncomputable, but can be approximated via empirical risk minimization:

$$f^*(x) = \arg\min_f \left\{ \frac{1}{n} \sum_{i=1}^{n} l(y_i, f(x_i)) \right\} . \tag{4}$$

The gap between the two approaches is called generalization gap.

# Overfitting

Consider the following algorithm (a variation of $1$-NN):

$$f(x) = \begin{cases} y & \text{if } (x, y) \in \mathcal{S}\,, \\ 0 & \text{otherwise}\ . \end{cases} \tag{5}$$

This has $0$ training error by construction, but a very large test error: this is an example of overfitting. We will see that (large) neural networks have many counter-intuitive properties when it comes to generalization.

# Some simplifications

To begin our exploration of supervised learning, we will make a few simplifying assumptions:

- The input $\mathbf{x}$ is a vector of shape $d$.
  $(d)$
- The output $y$ is a single real number.

There are three interesting cases: when $y \in \mathbb{R}$, it is a regression task; when $y \in \{0, \ldots, c-1\}$, it is a classification task; when $c = 2$, it is a binary classification task.

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# How to build a loss function?

Building a loss function can be done empirically: considering regression, for example, the prediction error $(y - \hat{y})$ is a reasonable quantity to penalize.
Since most times we do not care about the sign of the error, these are all valid choices:

$$\underbrace{(y-\hat{y})^2}_{\textbf{squared} \text{ loss}} \quad , \quad \underbrace{|y-\hat{y}|}_{\textbf{absolute} \text{ loss}} \quad , \quad \underbrace{\left(\log(1+y) - \log(1+\hat{y})\right)^2}_{\textbf{squared log loss}} \tag{6}$$

Is there a principled way to make the choice?

# Probabilistic formulation

Let us assume that $f(x)$ parameterizes a *probability distribution* $\hat{p}(y \mid f(x))$ over the possible outputs $y$. We are now choosing $\hat{p}(\cdot \mid \cdot)$ instead of $l(\cdot, \cdot)$, which can feel more natural.
For example, for regression we can assume a Gaussian shape:

$$\hat{p}(y \mid f(x)) = \mathcal{N}(y \mid f(x), \sigma^2)\,, \tag{7}$$

where the model predicts the center of a Gaussian distribution with fixed variance (hyper-parameter).

# Maximum likelihood

The probabilistic formulation also provides a principled way to interpret training by maximizing the likelihood (or log-likelihood) of the model (assuming the elements of the dataset are i.i.d.):

$$f^*(x) = \arg\max \prod_{(x_i, y_i)} \hat{p}(y_i \mid f(x_i)) = \arg\min \sum_{(x_i, y_i)} -\log \hat{p}(y_i \mid f(x_i)) \,. \tag{8}$$

Under the Gaussian assumption in (7), we obtain $-\log \hat{p}(y_i \mid f(x_i)) \propto (y_i - f(x_i))^2$, i.e., we should optimize the squared loss!

## 2 Linear models

Linear models for regression

Solving the LS problem

Overparameterized models and convergence (*optional*)

Linear models for classification

Calibration and a probabilistic formulation

# What is a linear model?

A linear model $f$ is defined as:

$$f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle = \mathbf{w}^\top \mathbf{x} = \sum_j w_j x_j \,, \tag{9}$$

where $\mathbf{w}$ is a vector of adaptable parameters.

This model is fundamental in many disciplines, ranging from econometrics to statistics.

# Linear models with bias

A more general formulation considers the inclusion of an offset (bias) $b \in \mathbb{R}$:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b\,. \tag{10}$$

Because we can always rewrite this as $\mathbf{w}^\top \bar{\mathbf{x}}$, with $\bar{\mathbf{x}} = [\mathbf{x};\ 1]$, we can avoid writing the bias explicitly to simplify the notation.

> **Hint**: Everytime we write a linear model, mentally add an offset term whenever needed.

# Graphical representation

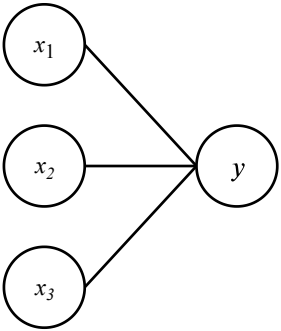



Figure 1: Each arrow represents a *linear* influence on the destination, which sums the results.

# Least-squares cost function

Combining the squared loss with a linear model results in the least-squares optimization problem:

$$\text{LS}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \mathbf{w}^\top \mathbf{x}_i\right)^2. \tag{11}$$

We can vectorize LS as:

$$\text{LS}(\mathbf{w}) = \frac{1}{n}\underset{(n)}{\left\|\ \mathbf{y}\ \right.} - \underset{(n,d)(d)}{\left.\ \mathbf{X}\ \ \mathbf{w}\right\|^2}, \tag{12}$$

where $[\mathbf{X}]_i = \mathbf{x}_i$ and $[\mathbf{y}]_i = y_i$.

## 2 Linear models

# Solving the LS problem

LS is a convex problem, with a simple gradient (normal equations):

$$\nabla \text{LS}(\mathbf{w}) = \frac{2}{n}\mathbf{X}^\top(\mathbf{X}\mathbf{w} - \mathbf{y})\,. \tag{13}$$

LS is special in the sense that $\nabla \text{LS}(\mathbf{w}) = 0$ is a linear equation that can be solved explicitly:

$$\mathbf{w}^* = \underset{(d,d)}{\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}}\underset{(d,n)(n)}{\mathbf{X}^\top\,\mathbf{y}} = \underset{(d,n)}{\mathbf{X}^\top}\underset{(n,n)}{\left(\mathbf{X}\mathbf{X}^\top\right)^{-1}}\underset{(n)}{\mathbf{y}}\,. \tag{14}$$

The terms $\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top$ and $\mathbf{X}^\top\left(\mathbf{X}\mathbf{X}^\top\right)^{-1}$ are called the pseudoinverses of $\mathbf{X}$, and they require the corresponding matrices to be invertible (full rank).

# Regularizing the LS problem

Numerical problems in the inversion of $\left(\mathbf{X}^\top \mathbf{X}\right)$ can be solved by adding a small amount of $\ell_2$ regularization (ridge regression):

$$\text{LS-REG}(\mathbf{w}) = \text{LS}(\mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|^2 , \tag{15}$$

for some $\lambda > 0$. This makes the problem *strictly* convex and forces the solution to be contained in a ball of given radius, modifying the gradient and the explicit solution as:

$$\nabla\text{LS-REG}(\mathbf{w}) = \nabla\text{LS}(\mathbf{w}) + \lambda\mathbf{w} . \tag{16}$$

$$\mathbf{w}^* = \left(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}\right)^{-1} \mathbf{X}^\top \mathbf{y} . \tag{17}$$

where $\mathbf{I}$ is the identity matrix of appropriate shape.

# Show me some code!

Generating some data:

```
# Linear model with unknown coefficients
X = torch.randn((10, 5))
y = X @ torch.randn((5, 1))
```

Computing a linear model:

```
w = torch.randn((5, 1))
yhat = X @ w # (10, 1)
```

Computing the objective function:

```
mse = ((y - X @ w)**2).mean()
```

# Show me some code (2)!

Explicit solution (numerically unstable):

```
1 wopt = torch.linalg.inv(X.T @ X) @ X.T @ y
```

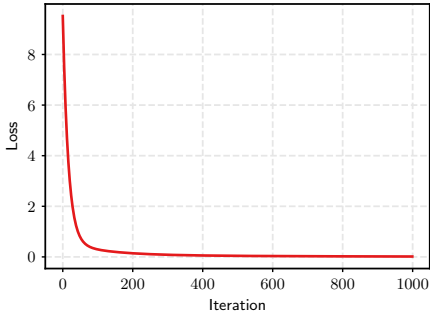
Explicit solution (better numerical conditioning):

```
1 wopt = torch.linalg.solve(X.T @ X, X.T @ y)
```

# Show me some code (3)!

Simple implementation of gradient descent:

```
loss = []
for i in range(1000):
loss.append(((y - X @ w)**2).mean().item())
# Note the sign: the derivative has a minus.
w = w + 0.001 * X.T @ (y - X @ w)
```



# Computational complexity of LS

Matrix multiplication $\underset{(a,b)(b,c)}{\mathbf{A}\ \mathbf{B}}$ has complexity $\mathcal{O}(abc)$, while matrix inversion has complexity (roughly) cubic.

For large models and datasets, we want algorithms that can scale linearly in both $n$ and $d$: we will see that gradient descent can satisfy this property.

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# Analyzing the convergence

Rewriting the GD step for the LS problem (ignoring the constant factor $2/n$):

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \eta \mathbf{X}^\top (\mathbf{X}\mathbf{w}_{t-1} - \mathbf{y}) \,. \tag{18}$$

We can use this to write out how the *predictions* over the training set evolve:

$$\hat{\mathbf{y}}_t = \hat{\mathbf{y}}_{t-1} - \eta \mathbf{X}\mathbf{X}^\top \left(\hat{\mathbf{y}}_{t-1} - \mathbf{y}\right) \,, \tag{19}$$

or, after some manipulation:

$$(\hat{\mathbf{y}}_t - \mathbf{y}) = \left(\mathbf{I} - \eta \mathbf{X}\mathbf{X}^\top\right) \left(\hat{\mathbf{y}}_{t-1} - \mathbf{y}\right) = \left(\mathbf{I} - \eta \mathbf{X}\mathbf{X}^\top\right)^t (\hat{\mathbf{y}}_0 - \mathbf{y}) \,. \tag{20}$$

See PPA, Chapter 5 for the full analysis.

# Overparameterized models

Eq. (20) is an interesting dynamical system: it will diverge in general, unless (a) all eigenvalues $\lambda_0, \ldots, \lambda_n$ of $\mathbf{X}\mathbf{X}^\top$ are non-negative, and (b) $\eta \in [0, 1/\lambda_0]$. In this case, it will decrease to $0$. If all eigenvalues are positive, it will do so *exponentially*.

For the latter condition, we need $d > n$, otherwise the matrix $\mathbf{X}\mathbf{X}^\top$ will have low-rank (hence, some zero eigenvalues). We call this the over-parameterized regime: it is possible in this case for LS to perfectly interpolate all training data exponentially fast!

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# Multi-class classification

In classification, $y$ is an integer $\{0, \ldots, c-1\}$, such that $y_i = j$ means that $\mathbf{x}_i$ is of class $j$.
For example, with $c = 3$ we might have:

- $y = 0$: the email is spam;
- $y = 1$: the email is legit;
- $y = 2$: the email is dubious.

Solving these as regression tasks is generally not an optimal choice: among other things, it is not guaranteed that classes have a definite ordering.

# Probability distributions

A common solution is to predict a probability distribution over the classes.

A vector $\mathbf{a}^{(c)}$ belongs to the probability simplex $\Delta_c$ if:

$$\sum_i [\mathbf{a}]_i = 1\,, \quad [\mathbf{a}]_i \geq 0\,. \tag{21}$$

If $f(\mathbf{x}) = \hat{\mathbf{y}} \in \Delta_c$, we can interpret it as a categorical probability distribution, e.g., we can select the class with highest probability as:

$$\text{class} = \arg\max_i [\hat{\mathbf{y}}]_i\,. \tag{22}$$

# A comment on differentiability

Note that we *cannot* easily predict an integer with our models, because it would require some form of threshold operation which is not compatible with gradient descent (gradient zero almost everywhere).
Predicting a probability distribution can be seen as a *soft* approximation to this problem.

# The softmax function

The softmax function maps any vector to the probability simplex:

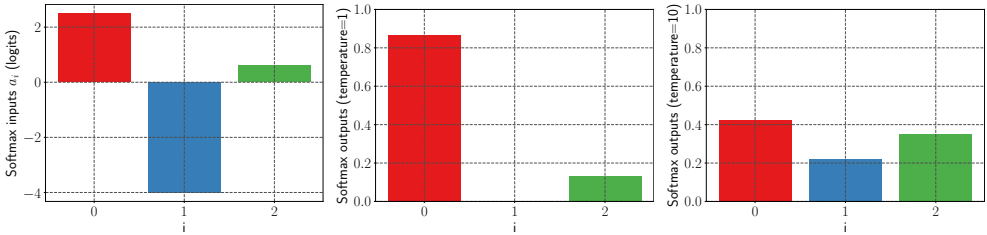
$$[\text{softmax}(\mathbf{a})]_i = \frac{\exp(a_i)}{\sum_j \exp(a_j)} \tag{23}$$

The numerator ensures that all outputs are positive, while the denominator ensures that the final vector sums to $1$. It can be seen as a soft approximation to the argmax (a better name is in fact *softargmax*).

If desired, we can control the approximation with an additional hyper-parameter $\tau$ called temperature:

$$[\text{softmax}(\mathbf{a})]_i = \frac{\exp(a_i/\tau)}{\sum_j \exp(a_j/\tau)} \tag{24}$$

# Visualizing the softmax function




(a) Softmax inputs (logits) (b) Softmax outputs (temperature = 1) (c) Softmax outputs (temperature = 10)

# Final model

Our linear model for classification becomes:

$$f(\mathbf{x})_{(c)} = \text{softmax}(\mathbf{W}_{(c,d)} \cdot \mathbf{x}_{(d)}) \tag{25}$$

The pre-softmax values $\mathbf{W}\mathbf{x}$ are called the logits of the model.

# One-hot encoding

In order to compare the predictions with the ground truth, we encode our targets using a one-hot encoding. Given a pair $(\mathbf{x}, \mathbf{y})$:

$$y_i = \begin{cases} 1 & \text{if } \mathbf{x} \text{ is of class } i\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{26}$$

For example, with $3$ classes $\{\text{cat}, \text{dog}, \text{other}\}$:

$$\text{cat} = [1, 0, 0] \quad \text{dog} = [0, 1, 0] \quad \text{other} = [0, 0, 1]\,. \tag{27}$$

This is a probability distribution putting all the **mass** on a single class.

# Cross-entropy loss

Finally, we need a loss function $l$ to compare two probability distributions.

The cross-entropy loss is defined for two vectors $\mathbf{y}, \hat{\mathbf{y}} \in \Delta_c$ as:

$$\text{CE}(\mathbf{y}, \hat{\mathbf{y}}) = -\sum_i y_i \log\left(\hat{y}_i\right) . \tag{28}$$

The CE loss can be derived from the maximum likelihood principle under the assumption that $f(\mathbf{x})$ encodes a categorical distribution (try it!).

# Logistic regression

A logistic regression is a linear model $f(\mathbf{x}) = \text{softmax}(\mathbf{W}\mathbf{x})$ trained by optimizing the cross-entropy:

$$\text{LR}(\mathbf{W}) = \frac{1}{n}\sum_{i=1}^{n} \text{CE}\left(\mathbf{y}_i, f(\mathbf{x}_i)\right) . \tag{29}$$

It is not possible to solve the logistic regression problem explicitly. A linear model for classification has $dc$ parameters.

# Binary classification

A special case is binary classification, where $c = 2$. In this case, we can predict a single scalar value $f(\mathbf{x}) \in [0, 1]$ since:

$$f(\mathbf{x}) \quad \text{probability of class 1} \ , \tag{30}$$

$$1 - f(\mathbf{x}) \quad \text{probability of class 2} \ . \tag{31}$$

The softmax function simplifies to the sigmoid function:

The sigmoid $\sigma(s) \in [0, 1]$ is defined as:

$$\sigma(s) = \frac{1}{1 + \exp(-s)} \, . \tag{32}$$

# Visualizing the sigmoid function

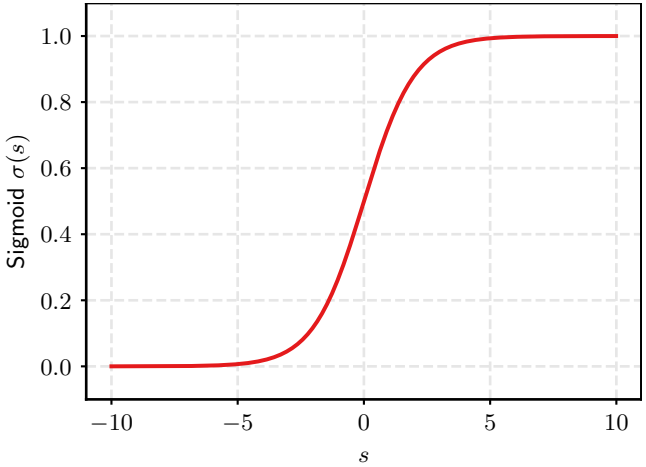



Figure 2: A visualization of the sigmoid function. Note that $0$ and $1$ are only approached asymptotically.

# Binary logistic regression model

Combining everything, we obtain a binary version of the logistic regression algorithm:

$$\text{BIN-LR}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}\Big[\underbrace{-y_i \log\big(\sigma(\mathbf{w}^\top \mathbf{x})\big)}_{\text{Class 1}} \underbrace{-(1-y_i)\log\big(1-\sigma(\mathbf{w}^\top \mathbf{x})\big)}_{\text{Class 2}}\Big] \tag{33}$$

In this case, we can obtain the most probable class from the model as:

$$\text{class} = \begin{cases} 0 & \text{if } \sigma(\mathbf{w}^\top \mathbf{x}) > 0.5\,, \\ 1 & \text{otherwise}\ . \end{cases} \tag{34}$$

# Gradient of the logistic regression

By manually differentiating we obtain:

$$\sigma'(s) = \sigma(s)(1 - \sigma(s))\,. \tag{35}$$

Plugging this into the gradient computation we obtain:

$$\nabla \text{BIN-LR}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(\sigma(\mathbf{w}^\top \mathbf{x}_i) - y_i)\mathbf{x}_i\,, \tag{36}$$

showing its similarity to the regression case.

# Implementation

```
from torch import nn

# Basic one: requires logits in input and indices or one-hot encodings for targets
torch.nn.CrossEntropyLoss()(ytrue, yhat)

# For this one, inputs should be the log of the softmax
torch.nn.NLLLoss()(ytrue, yhat)

# Specialized variants for binary cross-entropy
torch.nn.BCELoss()(ytrue, yhat)
torch.nn.BCEWithLogitsLoss()(ytrue, yhat)

# There are also functional variants
torch.nn.functional.cross_entropy(ytrue, yhat)
# ...
```

# The logsumexp function

Why a variant with logits in input? Note that the $i$th term of the cross-entropy wrt the logits $\mathbf{p}$ is given by:

$$-\log\left(\frac{\exp p_i}{\sum_j \exp p_j}\right). \tag{37}$$

In practice, this can be *highly* unstable. However, it can be rewritten as:

$$-p_i + \text{logsumexp}(\mathbf{p}), \tag{38}$$

where logsumexp is defined as $\text{logsumexp}(\mathbf{p}) = \log\left(\sum_i \exp p_i\right)$.

https://gregorygundersen.com/blog/2020/02/09/log-sum-exp/

# The logsumexp trick

The reason this is important is that the logsumexp function is invariant in the following sense:

$$\text{logsumexp}(\mathbf{p}) = \log\left(\sum_i \exp(p_i - c)\right) + c\,, \tag{39}$$

where $c$ is an arbitrary constant. By setting $c = \max(\mathbf{p})$, we can ensure numerical instabilities never occur.

In this sense, softmax can be interpreted as part of the model *or* as part of the loss; this is not an issue, since $\arg\max$ only cares about the relative ranking of the values, which is not changed by the softmax.

## 2 Linear models

# Calibration

A common misconception when doing classification is that $[f(x)]_i$ can be immediately interpreted as *the probability of pattern $x$ being of class $i$*.
However, this is only true whenever the trained model satisfies:

$$p(y = i \,|\, x) = [f(x)]_i \,. \tag{40}$$

We say the model is well calibrated, but this must be checked manually.

Guo, C., et al.. **On calibration of modern neural networks**. ICML 2017.

# Measuring calibration

To measure the calibration of a model, we keep a separate validation set, and we split the interval $[0, 1]$ into $m$ equispaced bins (each of size $1/m$). Define:

- $B_m$ the number of samples from the validation set, whose predicted confidence falls in bin $m$.
- $p_m$ the average confidence of the network for that bin.
- $a_m$ the average accuracy of the network for these elements.

Then, the expected calibration error (ECE) is given by:

$$\text{ECE} = \sum_m \frac{B_m}{n} |a_m - p_m| \,. \tag{41}$$

# Calibration plots

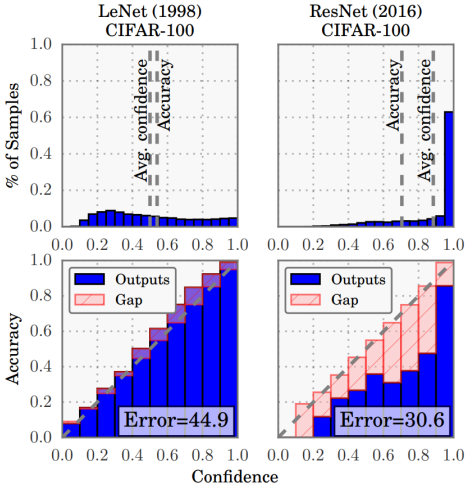



Figure 3: Plotting $a_m$ against $p_m$ for every bin gives us a reliability plot (from Guo et al., 2017).

# Focal loss

This topic is important because more complex networks may be highly over (or under) confident, with many methods to improve it (temperature scaling, logit normalization, ...).
A simple (and popular) option is to decrease the weight given to 'easy' samples using a variant of cross-entropy call the focal loss:

$$\text{FL}_\alpha(\mathbf{y}, \hat{\mathbf{y}}) = -(1 - \hat{\mathbf{y}}_c)^\alpha \log \hat{\mathbf{y}}_c \,, \tag{42}$$

where $c = \arg\max \mathbf{y}$.

Mukhoti, J., et al., 2020. **Calibrating deep neural networks using focal loss**. *Advances in Neural Information Processing Systems*, 33, pp. 15288-15299.

# Visualizing the focal loss

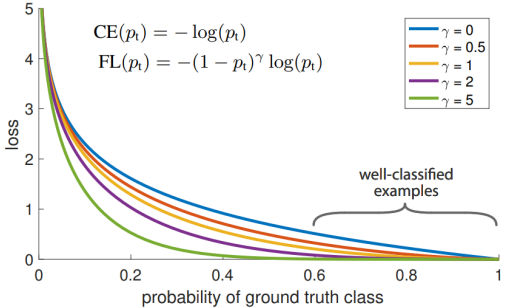



Figure 1. We propose a novel loss we term the *Focal Loss* that adds a factor $(1 - p_t)^{\gamma}$ to the standard cross entropy criterion. Setting $\gamma > 0$ reduces the relative loss for well-classified examples ($p_t > .5$), putting more focus on hard, misclassified examples. As

Lin, T.Y., et al., 2017. **Focal loss for dense object detection**. In *IEEE ICCV* (pp. 2980-2988).

# Reading material

- **Dive into Deep Learning**: Chapters 3 and 4.