Deep learning

2.1. Loss and risk

François Fleuret

https://fleuret.org/dlc/

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The general objective of machine learning is to capture regularity in data to make predictions.

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There are multiple types of inference that we can roughly split into three categories:

- Classification (e.g. object recognition, cancer detection, speech processing),
- regression (e.g. customer satisfaction, stock prediction, epidemiology), and
- density estimation (e.g. outlier detection, data visualization, sampling/synthesis).
The standard formalization considers a measure of probability

$$\mu_{X,Y}$$

over the observation/value of interest, and i.i.d. training samples

$$(x_n, y_n), \ n = 1, \ldots, N.$$
Intuitively, for classification it can often be interpreted as

$$\mu_{X,Y}(x,y) = \mu_{X|Y=y}(x) P(Y = y)$$

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So the quantity

$$\mu_{X|Y=y}$$

stands for the distribution of the observable signal for the class $y$ (e.g. “sound of an /e/”, “image of a cat”).
For regression, one would interpret the joint law more naturally as

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In the simple cases

$$Y = f(X) + \epsilon$$

where $f$ is the deterministic dependency between $x$ and $y$, and $\epsilon$ is a random noise, independent of $X$. 
With such a probabilistic perspective, we can more precisely define the three types of inferences we introduced before:

**Classification,**
- \((X, Y)\) random variables on \(\mathcal{X} = \mathbb{R}^D \times \{1, \ldots, C\}\),
- we want to estimate \(\arg\max_y P(Y = y \mid X = x)\).
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**Regression,**

- $(X, Y)$ random variables on $\mathcal{F} = \mathbb{R}^D \times \mathbb{R}$,
- we want to estimate $\mathbb{E}(Y \mid X = x)$.
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**Density estimation,**
- \(X\) random variable on \(\mathcal{X} = \mathbb{R}^D\),
- we want to estimate \(\mu_X\).
The boundaries between these categories are fuzzy:

- Regression allows to do classification through class scores.
- Density models allow to do classification thanks to Bayes’ law.

etc.
Risk, empirical risk
Learning consists of finding in a set $\mathcal{F}$ of functionals a “good” $f^*$ (or its parameters’ values) usually defined through a loss

$$\ell: \mathcal{F} \times \mathcal{Z} \to \mathbb{R}$$

such that $\ell(f, z)$ increases with how wrong $f$ is on $z$. 
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- for classification:
  $$\ell(f, (x, y)) = \mathbf{1}_{\{f(x) \neq y\}},$$

- for regression:
  $$\ell(f, (x, y)) = (f(x) - y)^2,$$

- for density estimation:
  $$\ell(q, z) = -\log q(z).$$
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- for classification:
  $$\ell(f, (x, y)) = 1_{\{f(x) \neq y\}},$$

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- for density estimation:
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The loss may include additional terms related to $f$ itself.
We are looking for an $f$ with a small **expected risk**

$$R(f) = \mathbb{E}_Z (\ell(f, Z)),$$

which means that our learning procedure would ideally choose

$$f^* = \arg\min_{f \in \mathcal{F}} R(f).$$
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Although this quantity is unknown, if we have i.i.d. training samples

$$\mathcal{D} = \{Z_1, \ldots, Z_N\},$$

we can compute an estimate, the **empirical risk**:

$$\hat{R}(f; \mathcal{D}) = \hat{\mathbb{E}}_{\mathcal{D}} (\ell(f, Z)) = \frac{1}{N} \sum_{n=1}^{N} \ell(f, Z_n).$$
We have

$$\mathbb{E}_{Z_1, \ldots, Z_N} \left( \hat{R}(f; \mathcal{D}) \right) = \mathbb{E}_{Z_1, \ldots, Z_N} \left( \frac{1}{N} \sum_{n=1}^{N} \ell(f, Z_n) \right)$$
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The empirical risk is an unbiased estimator of the expected risk.
Finally, given $\mathcal{D}$, $\mathcal{F}$, and $\ell$, “learning” aims at computing

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- Can we bound $R(f)$ with $\hat{R}(f; \mathcal{D})$?

Yes if $f$ is not chosen using $\mathcal{D}$. Since the $Z_n$ are independent, we just need to take into account the variance of $\hat{R}(f; \mathcal{D})$. 

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  Unfortunately not simply, and not without additional constraints on $\mathcal{F}$.

  For instance if $|\mathcal{F}| = 1$, we can!
Note that in practice, we call “loss” both the functional

$$\ell : \mathcal{F} \times \mathcal{L} \to \mathbb{R}$$

and the empirical risk minimized during training

$$\mathcal{L}(f) = \frac{1}{N} \sum_{n=1}^{N} \ell(f, z_n).$$
The end