Invariance reduces Variance: Understanding Data Augmentation in Deep Learning and Beyond

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Abstract

Many complex deep learning models have found success by exploiting symmetries in data. Convolutional neural networks (CNNs), for example, are ubiquitous in image classification due to their use of translation symmetry, as image identity is roughly invariant to translations. In addition, many other forms of symmetry such as rotation, scale, and color shift are commonly used via data augmentation: the transformed images are added to the training set. However, a clear framework for understanding data augmentation is not available. One may even say that it is somewhat mysterious: how can we increase performance by simply adding transforms of our data to the model? Can that be information theoretically possible?

In this paper, we develop a theoretical framework to start to shed light on some of these problems. We explain data augmentation as averaging over the orbits of the group that keeps the data distribution invariant, and show that it leads to variance reduction. We study finite-sample and asymptotic empirical risk minimization (using results from stochastic convex optimization, Rademacher complexity, and asymptotic statistical theory). We work out as examples the variance reduction in exponential families, linear regression, and certain two-layer neural networks under shift invariance (using discrete Fourier analysis). We also discuss how data augmentation could be used in problems with symmetry where other approaches are prevalent, such as in cryo-electron microscopy (cryo-EM).

1 Introduction

Deep learning algorithms such as convolutional neural networks (CNNs) are successful in part because they exploit natural symmetry in the data. For instance, image identity is roughly invariant to translations and rotations: so a slightly translated cat is still a cat. Such invariances are present in many datasets,

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Figure 1: An image of a slightly translated cat remains a cat. This invariance is used in data augmentation, by training models not just with the original data, but also with the transformed data. We show that this can be viewed as averaging over group orbits, and hence reduces variance.
including image, text and speech data. Standard architectures are invariant to some, but not all transforms. For instance, CNNs induce an approximate equivariance to translations, but not to rotations. This is the inductive bias of CNNs, and the idea dates back at least to the neocognitron (Fukushima, 1980).

To make models invariant to arbitrary transforms beyond the ones built into the architecture, data augmentation is commonly used. Roughly speaking, the model is trained not just with the original data, but also with transformed data. Data augmentation is a crucial component of modern deep learning pipelines, and it is typically needed to achieve state of the art performance. It has been used e.g., in AlexNet (Krizhevsky et al., 2012), and other pioneering works (Ciresan et al., 2010). See Figure 2 for a small experiment (see Section 6.2 for details).

Equivariant or invariant architectures (such as CNNs) are attractive for tackling invariance. However, in many cases, datasets have symmetries that are naturally described in a generative form: we can specify generators of the group of symmetries (e.g., rotations and scalings). In contrast, computing the equivariant features requires designing new architectures. Thus, data augmentation is a universally applicable, generative, and algorithmic way to exploit invariances.

However, a general framework for understanding data augmentation is missing. Such a framework would enable us to reason clearly about the benefits offered by augmentation, in comparison to invariant features. Moreover, such a framework could also shed light on perhaps mysterious questions such as: How can we improve the performance of our models by simply adding transformed versions of the training data? Doesn’t that contradict basic statistical principles? However, developing such a framework is challenging for several reasons: first, it is unclear what mathematical approach to use, and second it is unclear how to demonstrate that data augmentation “helps”.

In this paper we propose such a general framework. We use group theory as a mathematical language, and model invariances as equality in distribution (or small changes in distribution) under a group action. We show that data augmentation can be viewed as invariant learning by averaging over the group action. We then demonstrate that data augmentation leads to sample efficient learning, both in the non-asymptotic setting (relying on results from stochastic convex optimization and Rademacher complexity), as well as in the asymptotic setting (by using asymptotic statistical theory for empirical risk minimizers/M-estimators).

We show how to apply data augmentation beyond deep learning, to other problems in statistics and machine learning that have invariances. In addition, we explain the connections to several other important notions from statistics and machine learning, including sufficiency, invariant representations, equivariance, variance reduction in Monte Carlo methods, and regularization. We also review related works. Here we mention one of the most related works, Bloem-Reddy and Teh (2019), who use similar probabilistic models, but without focusing on data augmentation.

We can summarize our main contributions as follows:
1. We study data augmentation in a group-theoretic formulation, where there is a group acting on the data, and the distribution of the data is equal (or does not change too much) under the action. We explain that in empirical risk minimization (ERM) this leads to minimizing an augmented loss, which is the average of the original loss under the group action (Section 3.1). We also propose to extend data augmentation beyond ERM, using the "augmentation distribution" (Section 3.3).

2. We provide several theoretical results to support the benefits of data augmentation. When the data is exactly invariant in distribution, we show that averaging over the group orbit (e.g., all rotations) reduces the variance of any function, including the loss and the gradients of the loss. We can immediately conclude that estimators based on the "augmentation distribution" gain efficiency and augmentation reduces the mean squared error (MSE) of general estimators (Section 4.1).

Moving to the more specialized case of empirical risk minimizers, we show that as a consequence of the above, data augmentation reduces variance in ERM (Section 4.2.1). Here we use very recent results from stochastic convex optimization. We also show that data augmentation reduces the Rademacher complexity of a loss class (Section 4.2.2). Notably, this last result allows the distribution of the transformed data to be different from the original data, and the bound depends on a specific Wasserstein distance between the two.

3. Moving to the asymptotic case, we characterize the precise variance reduction obtained by data augmentation. We show that this depends on the covariance of the loss gradients along the group orbit (Section 4.2.3). This implies that data augmentation can improve upon the Fisher information of the un-augmented maximum likelihood estimator (MLE) (Section 4.2.4). We study the special case when the subspace of parameters with invariance is a low-dimensional manifold (Section 4.2.5). We connect this to geometry showing that the projection of the gradient into the tangent space is always invariant; however it does not always capture all invariance.

4. We work out several examples of our theory (Section 5): exponential families, nonlinear regression and two-layer neural networks with circular shift data augmentation in the heavily underparametrized regime (where most of our results concern quadratic activations), nonlinear least squares classification with circular shifts, and linear regression with general linear group actions.

We also describe a few important problems where symmetries occur, but where other approaches—not data augmentation—are currently used: cryo-electron microscopy (cryo-EM), spherically invariant data, and random effects models. These problems may be especially promising for using data augmentation.

2 Some related work

In this section we discuss some related works, in addition to those that are mentioned in other places.

Data augmentation methodology in deep learning. There is a great deal of work in developing efficient methods for data augmentation in deep learning. Here we briefly mention a few works. Data augmentation has a long history, and related ideas date back at least to Baird (1992), who built a "pseudo-random image generator", that "given an image and a set of model parameters, computes a degraded image". This is recounted in Schmidhuber (2015).

Conditional generative adversarial networks (cGAN) are a method for learning to generate from the class-conditional distributions in a classification problem (Mirza and Osindero, 2014). This has direct applications to data augmentation. Data augmentation GANs (DAGAN) (Antoniou et al., 2017) are a related approach that train a GAN to discriminate between $x, x_g$, and $x, x'$, where $x_g$ is generated as $x_g = f(x, z)$, and $x'$ is an independent copy. This learns the conditional distribution $x' | x$, where $x', x$ are sampled "independently" from the training set. Here the training data is viewed as non-independent and they learn the dependence structure.

Hauberg et al. (2016) construct class-dependent distributions over diffeomorphisms for learned data augmentation. Ratner et al. (2017) learn data augmentation policies using reinforcement learning, starting with a known set of valid transforms. Tran et al. (2017) propose a Bayesian approach. RenderGAN (Sixt et al., 2018) combines a 3D model with GANs for image generation. DeVries and Taylor (2017a) propose
to perform data augmentation in feature space. AutoAugment (Cubuk et al., 2018) is another approach for learning augmentation policies based on reinforcement learning, which is one of the state of the art approaches.

**Neural net architecture design.** There is a parallel line of work designing invariant and equivariant neural net architectures. A key celebrated example is convolutions, dating back at least to the neocognitron (Fukushima, 1980), see also LeCun et al. (1989). More recently, group equivariant Convolutional Neural Networks (G-CNNs), have been proposed, using G-convolutions to exploit symmetry (Cohen and Welling, 2016a). That work designs concrete architectures for groups of translations, rotations by 90 degrees around any center of rotation in a square grid, and reflections. Dieleman et al. (2016) designed architectures for cyclic symmetry.

Worrall et al. (2017) introduce Harmonic Networks or H-Nets, which induce equivariance to patch-wise translation and 360 degree rotation. They rely on circular harmonics as invariant features. Cohen and Welling (2016b) propose steerable CNNs and Cohen et al. (2018a) develop a more general approach. There are several works on SO(3) equivariance, see Cohen et al. (2018b); Esteves et al. (2018a,b, 2019).

Gens and Domingos (2014) introduce deep symmetry networks (symnets), that form feature maps over arbitrary symmetry groups via kernel-based interpolation to pool over symmetry spaces. See also Ravabakhsh et al. (2017); Kondor and Trivedi (2018); Weiler et al. (2018); Kondor et al. (2018). There are also many examples of data augmentation methods developed in various application areas, e.g., Jaitly and Hinton (2013); Xie et al. (2019); Park et al. (2019); Ho et al. (2019), etc.

**Data augmentation as a form of regularization.** There is also a line of work proposing to add random or adversarial noise to the data when training neural networks. The heuristic behind this approach is that the addition of noise-perturbed data should produce a classifier which is robust to random or adversarial corruptions.

For example, DeVries and Taylor (2017b) proposes to randomly mask out square regions of input images and fill the regions with pure gray color; Zhong et al. (2017) and Lopes et al. (2019) propose to randomly select a patch within an image and replace its pixels with random values; Bendory et al. (2018) proposes to add Perlin noise (Perlin, 1985) to medical images; Zhang et al. (2017) proposes to train with convex combinations of two images as well as their labels. The experiments done by those papers show that augmenting with noise-perturbed data can lead to lower generalization error and better robustness against corruptions.

Szegedy et al. (2013) and Cohen et al. (2019) demonstrate that training with adversarial examples can lead to some form of regularization. Hernández-García and König (2018a) has argued that data augmentation can sometimes even replace other regularization mechanisms such as weight decay, while Hernández-García and König (2018b) has argued that this can be less sensitive to hyperparameter choices than other forms of regularization.

While this approach is also called data augmentation in the literature, it is fundamentally different from what we consider. We study a way to exploit invariance in the data, while those works focus on smoothing effects (adding noise cannot possibly lead to exactly invariant distributions).

**Other works connected to data augmentation.** There is a tremendous amount of other work connected to data augmentation. On the empirical end, Bengio et al. (2011) have argued that the benefit of data augmentation goes up with depth. On the theoretical end Rajput et al. (2019) investigate if gaussian data augmentation leads to positive margin, with some negative results. Connecting to adversarial examples, Engstrom et al. (2017) show that adversarially chosen group transforms such as rotations can already be enough to fool neural network classifiers. Javadi et al. (2019) show that data augmentation can reduce a certain Hessian-based complexity of neural networks. Liu et al. (2019) show that data augmentation can significantly improve the optimization landscape of neural networks, so that SGD avoids bad local minima and leads to much more accurate trained networks. Hernández-García et al. (2018) has shown that it also leads to better biological plausibility in some cases.

Dao et al. (2019) also seek to establish a theoretical framework for understanding data augmentation, but focus on the connection between data augmentation and kernel classifiers. Dao et al. (2019) study k-NN and kernel methods. They show how data augmentation with a kernel classifier yields approximations which look like feature averaging and variance regularization, but do not explicitly quantify how this improves classification.

We also note that data augmentation has another meaning in Bayesian statistics, namely the introduction of auxiliary variables to help compute the posterior (see e.g., Tanner and Wong, 1987). The naming clash is
unfortunate. However, since the term “data augmentation” is well established in deep learning, we decided to keep it in our current work.

**Group invariance in statistical inference.** There has been significant work on group invariance in statistical inference (e.g., Giri, 1996). However the questions investigated there are different from the ones that we study. Among other contributions, Helland (2004) argues that group invariance can form natural non-informative priors for the parameters of the model, and introduces permissible sub-parameters as those upon which group actions can be defined.

**Physical invariances.** There is a long history of studying invariance and symmetry in physics. Invariances lead to conservation laws, such as conservation of mass and momentum. In additions, invariances in Hamiltonians of physical systems lead to reductions in the number of parameters of probability distributions governing the systems. This has been among the explanations proposed of why deep learning works (Lin et al., 2017).

### 3 Methodology for Data Augmentation

#### 3.1 ERM

We start by explaining our framework in the context of empirical risk minimization (ERM).

Consider observations \( X_1, \ldots, X_n \in \mathbb{R}^d \) (e.g., images) sampled i.i.d. from a probability distribution \( P \). Data augmentation is a way of “teaching invariance to the model”. We assume our data is invariant to certain transformations. Consider thus a group \( G \) acting on the sample space, e.g., rotations of images. We assume the following invariance structure. For any group element \( g \in G \), we have the equality in distribution

\[ X =_d gX. \]

Therefore, the distribution of \( X \) is invariant under the group action \( G \). Formally we have a group action \( \phi : G \times X \to X \), which acts on \( x \in \mathbb{R}^d \) via \( g \in G \) to produce \( \phi(g, x) = gx \).

For supervised learning applications, \( X_i = (Z_i, Y_i) \) contains both the features \( Z_i \) and the outcome \( Y_i \). For instance, this assumption can mean that the probability of an image being a bird is the same as the probability for a rotated image. This is a convenient approximation, and it is interesting to see how it can be extended to “approximate invariance”. Some of our approach applies to that case, see Section 4.2.2.

In this context, data augmentation corresponds to “adding all datapoints \( gX_i, g \in G, i = 1, \ldots, n \)” to the dataset. When the group is finite, this can effectively be implemented by enlarging the data size. However, many important groups are infinite, and to understand data augmentation in that setting, it is most clear if we argue from first principles.

**Data augmentation for ERM.** In practice, data augmentation is performed via the following approach. To start, we consider a loss function \( L(\theta, X) \), and attempt to minimize the empirical risk

\[ \min_{\theta} R_n(\theta) := \frac{1}{n} \sum_{i \in [n]} L(\theta, X_i). \] (1)

This objective is minimized iteratively over time \( t = 1, 2, \ldots \) by stochastic gradient descent (SGD), or variants. A small random subset—a minibatch—of \( X_i \) is chosen at every iteration (say with indices \( S_t \)). To each chosen datapoint, a random augmentation \( g_{R(i,t)} \) is applied. Here we need a probability distribution \( Q \) on the group \( G \), so \( g_{R(i,t)} \sim Q \) (and we will be more precise later). Then, the parameter is updated as

\[ \theta \leftarrow \theta - \frac{\eta}{|S_t|} \sum_{i \in S_t} \nabla L(\theta, g_{R(i,t)}X_i). \] (2)

A key observation is that this corresponds to SGD on an augmented empirical risk, where we take an average over all augmentations according to the measure \( Q \):

\[ \min_{\theta} R_{n,A}(\theta) := \frac{1}{n} \sum_{i \in [n]} \int L(\theta, gX_i) dQ(g). \] (3)
To be precise, \( \nabla L(\theta, g_{R(i,t)}X_i) \) is an unbiased stochastic gradient for the loss function \( \int L(\theta, gX_i)dQ(g) \). We can view the above estimator as an empirical risk minimizer with a new \textit{augmented} loss function
\[
\tilde{L}(\theta, X) = \int L(\theta, gX)dQ(g).
\]

This can be viewed as Rao-Blackwellizing the loss, meaning taking a conditional expectation of the loss over the conditional distribution of \( x \) belonging to the group orbits, i.e., \( x \in G \cdot x \). See Section 3.4 for more discussion.

**Parametric model.** We will resort to a a parametric statistical model \( \{\mathbb{P}_\theta, \theta \in \Theta\} \), where \( \Theta \subseteq \mathbb{R}^p \) is some parameter space. At the outset, we assume that the invariance condition \( X =_d gX \) holds for the true parameter \( \theta_0 \) only. However, it may hold for a larger subset of the parameter space.

A strength of our approach is the generality of the invariance structures we can allow. However, this requires some care to formulate properly. Formally, let us consider a locally compact Hausdorff group \( G \) with its Borel \( \sigma \)-algebra. Let \( Q(g) \) be a Haar probability measure on \( G \): for any \( g \in G \) and measurable \( S \subseteq G \), we require
\[
Q(gS) = Q(S), \quad Q(Sg) = Q(S).
\]

We then need the invariance to hold for \( Q \text{-a.e. } g \). However in the following we will still assume for simplicity that it holds for all \( g \). In terms of the density of the random variables with respect to some common \( \sigma \)-finite measure (when such densities exist), this can be written as: for \( \mathbb{P}_{\theta_0} \text{-a.e. } x \) and \( Q \text{-a.e. } g \), we have
\[
p_{\theta_0}(gx) \cdot \det Jacc(gx \to x) = p_{\theta_0}(x).
\]

**MLE.** The usual maximum likelihood estimation (MLE) approach goes as follows. Let \( p_{\theta} \) be the density of \( \mathbb{P}_{\theta} \) with respect to some \( \sigma \)-finite measure \( \mu \) on \( \mathbb{R}^d \). We define the log-likelihood function as \( \ell_{\theta}(x) = \log p_{\theta}(x) \). We then define the MLE as any solution of the following problem:
\[
\hat{\theta}_{\text{MLE},n} = \arg \max_{\theta \in \Theta} \sum_{i \in [n]} \ell_{\theta}(X_i).
\]

If the log-likelihood is not concave, here and in what follows we write \( \hat{\theta} \in \arg \max \), and take any maximizer.

**Constrained MLE.** The invariance structure is a constraint on the density function. Hence we obtain a natural \textit{constrained} (or restricted) maximum likelihood estimation problem. Define \( \Theta_G = \{\theta \in \Theta : X =_d gX, \forall g \in G\} \). Then the constrained MLE is
\[
\hat{\theta}_{\text{MLE},n} = \arg \max_{\theta \in \Theta_G} \sum_{i \in [n]} \ell_{\theta}(X_i).
\]

In general, this can be much more sample-efficient than the original MLE. For instance, suppose we are trying to estimate a normal mean based on one sample: \( X \sim \mathcal{N}(\theta, 1) \). Let the group be negation, i.e., \( G = \{\pm 1\}, \cdot = \mathbb{Z}_2 \). Then \( \Theta_G = \{0\} \), because the only normal density symmetric around zero is the one with zero mean. Hence, the invariance condition uniquely identifies the parameter, showing that the constrained MLE perfectly recovers the parameter.

However, in general optimizing over the restricted parameter set may be computationally more difficult. This is indeed the case in the applications we have in mind. For instance, in deep learning, \( G \) may correspond to the set of all translations, rotations, scalings, shearings, color shifts, etc. In reality, we do not exactly have a group, as we also have non-invertible transforms like image crops. However, for simplicity we will first work assuming the transforms have a group structure.

A particular example of the augmented ERM is augmented maximum likelihood estimation. Here the loss is the negative log-likelihood, \( L(\theta, x) = -\ell_{\theta}(x) \). Then the augmented maximum likelihood program becomes
\[
\hat{\theta}_{a\text{MLE},n} = \arg \max_{\theta \in \Theta_G} \sum_{i \in [n]} \int_G \ell_{\theta}(gx_i)dQ(g).
\]

**Invariant representations.** Another perspective to exploit invariance is that of invariant representations, i.e., learning over representations \( T(x) \) of the data such that \( T(gx) = T(x) \) (see also Section 3.4.2). However, it turns out that in some natural examples, the invariant MLE does not gain over the usual MLE (see also Section 6.1). Thus we will not consider this in much detail.
Table 1: Optimization objectives

| Objective             | Sample                                                                                   | Population                                                                 |
|-----------------------|------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|
| ERM                   | $\min_{\theta \in \Theta} \frac{1}{n} \sum_{i \in [n]} L(\theta, X_i)$                | $\min_{\theta \in \Theta} \mathbb{E}_\theta L(\theta, X)$                 |
| Invariant ERM         | $\min_{\theta \in \Theta} \frac{1}{n} \sum_{i \in [n]} L(\theta, T(X_i)), \quad T(x) = T(gx)$ | $\min_{\theta \in \Theta} \mathbb{E}_\theta L(\theta, T(X))$              |
| Constrained ERM       | $\min_{\theta \in \Theta, g} \frac{1}{n} \sum_{i \in [n]} L(\theta, X_i)$             | $\min_{\theta \in \Theta} \mathbb{E}_\theta L(\theta, X)$                 |
| Augmented ERM         | $\min_{\theta \in \Theta} \frac{1}{n} \sum_{i \in [n]} \int L(\theta, gX_i) dQ(g)$   | $\min_{\theta \in \Theta} \mathbb{E}_\theta \int L(\theta, gX) dQ(g)$     |

3.2 Marginal MLE

There is a natural additional method to estimate the parameters, the marginal MLE. Our original local invariance assumption is equivalent to the following latent variable model. Under the true parameter $\theta_0$, we sample a random group element $g \sim Q$, and a random datapoint $\tilde{X} \sim \mathbb{P}_{\theta_0}$, i.e.,

$$\tilde{X} \sim \mathbb{P}_{\theta_0}, \quad g \sim Q.$$

Then, we observe $X = g\tilde{X}$. We repeat this independently over all datapoints to obtain all $X_i$. Since $gX_i = gX$ under $\theta_0$, this sampling process is exactly equivalent to the original model, under $\theta_0$.

Suppose that instead of fitting this model, we attempt to fit the relaxed model

$$\tilde{X} \sim \mathbb{P}_{\theta}, \quad g \sim Q,$$

observing $X = g\tilde{X}$. The only change is that we assume that the invariance holds for all parameter values. This model is mis-specified, nonetheless it may be easier to fit computationally. Moreover its MLE may still retain consistency for the original true parameter. Now the maximum marginal likelihood estimator (ignoring terms constant with respect to $\theta$) can be written as:

$$\hat{\theta}_{mMLE,n} = \arg \max_{\theta} \sum_{i \in [n]} \log \left( \int_G p_\theta(gX_i) dQ(g) \right).$$

We emphasize that this is not the same as the augmented MLE estimator considered above. This estimator has the log($\cdot$) terms outside the $G$-integral, while the augmented one effectively has the log($\cdot$) terms inside.

Summary of methods. Thus we now have several estimators for the original problem: ERM, constrained ERM, augmented ERM (each of which can be specialized to MLE), and marginal MLE. See Table 1. Can we understand them? In the next sections we will develop theoretical results to address these questions.

3.3 Beyond ERM

The above ideas apply to empirical risk minimization. However, there are many popular algorithms and methods that are not most naturally expressed as plain ERM. For instance:

1. Regularized ERM, e.g., Ridge regression and Lasso
2. Shrinkage estimators, e.g., Stein shrinkage
3. Nearest neighbors, e.g., k-NN classification and regression
4. Heuristic algorithms like Forward stepwise (stagewise, streamwise) regression, and backward stepwise.

While these may be associated with an objective function, there may be no known computationally efficient methods for finding global solutions.
Consider therefore a general estimator \( \hat{\theta}(x) \) based on data \( x \). How can we do data augmentation? The simplest idea would be to try to compute the estimator on all the data, including the actual and transformed sets. Following the previous logic, if we have the invariance \( X = _d gX \) for all \( g \in G \), then after observing data \( x \), we should "augment" our data with \( gx \), for all \( g \in G \). Then we should run our method on this data. However, this idea is can be impractical, as the entire data can be too large to work with directly. Therefore, we will take a more principled approach and work through the logic step by step, considering all possibilities. We will eventually recover the above estimator as well.

**Augmentation distribution & General augmentations.** We define the augmentation distribution as the set of values

\[
\hat{\theta}(gx), \ g \in G.
\]

We think of \( x = (x_1, \ldots, x_n) \) as the entire dataset, and of \( g \in G \) being a group element summarizing the action on every datapoint. The augmentation distribution is simply the collection of values of the estimator we would get if we were to apply all group transforms to the data. It has a special role, because we think of each transform as equally informative, and thus each value of the augmentation distribution is an equally valid estimator.

We can also make this a proper probability distribution by taking a random \( g \sim Q \). Then we can construct a final estimator by computing a summary statistic on this distribution, for instance the mean

\[
\hat{\theta}_G(x) = \mathbb{E}_{g \sim Q} \hat{\theta}(gx).
\]

It is worth noticing that this definition is exactly invariant, so that \( \hat{\theta}_G(x) = \hat{\theta}_G(gx) \). Moreover, this estimator can be approximated in the natural way in practice via sampling \( g_i \sim Q \) independently:

\[
\hat{\theta}_k(x) = \frac{1}{k} \sum_{i=1}^{k} \hat{\theta}(g_ix).
\]

We will later study finite augmentations, and show that they retain some of the desired variance reduction properties.

**Connection to previous approach.** To see how this connects to the previous ideas, let us consider \( X = (X_1, \ldots, X_n) \), and \( \hat{\theta} \) be the ERM with loss function \( L(\theta, \cdot) \) from equation (1). Consider the group \( G^n = G \times \ldots \times G \) acting on \( X \) elementwise. Then, the augmentation distribution is the set of values

\[
\hat{\theta}(X_1, \ldots, X_n; g_1, \ldots, g_n) := \arg\min_{\theta} \frac{1}{n} \sum_{i \in [n]} L(\theta, g_i X_i).
\]

Then, the final estimator would be

\[
\hat{\theta}_G(X_1, \ldots, X_n) := \mathbb{E}_{g_1, \ldots, g_n \sim Q} \arg\min_{\theta} \frac{1}{n} \sum_{i \in [n]} L(\theta, g_i X_i).
\]

Compared to the previous augmented ERM estimator, the current one changes the order of averaging over \( G \) and minimization. Specifically, the previous one is \( \arg\min \mathbb{E}_G R_n(\theta; gX) \), while the current one is \( \mathbb{E}_G \arg\min R_n(\theta; gX) \). If we know that the estimator is obtained from minimizing a loss function, then we can average that loss function; but in general we can only average the estimator, which justifies the current approach.

The two approaches above closer than one may think. We can view the SGD iteration (2) as an online optimization approach to minimize a randomized objective of the form \( \sum_{i \in [n]} L(\theta, g_i X_i) \). This holds exactly if we take one pass over the data in a deterministic way, which is known as a type of incremental gradient method. In this case, minimizing the augmented ERM has a resemblance to minimizing the mean of the augmentation distribution. However, in practice people take multiple passes over the data, so this interpretation is not exact.

**Augmentation in sequence of estimators.** In the above generalization of data augmentation beyond ERM, we assumed only the bare minimum, meaning that the estimator \( \hat{\theta}(x) \) exists. Suppose now that we have slightly more structure, and the estimator is part of a sequence of estimators \( \hat{\theta}_n \), defined for all \( n \).
This is a mild assumption, as in general estimators can be embedded into sequences defined for all data sizes. Then we can directly augment our dataset $X_1, \ldots, X_n$ by adding new datapoints. We can define augmented estimators in several ways. For instance, for any fixed $m$, we can compute the estimator on uniformly resampled set of size $m$ from the data, applying uniform random transforms:

$$\hat{\theta}_m(g_1X_{i_1}, g_2X_{i_2}, \ldots, g_mX_{i_m})$$

$$i_k \sim \text{Uniform}[n], \ g_k \sim Q(g).$$

This implicitly assumes a form of symmetry of the estimator with respect to its arguments. There are many variations: e.g., we may insist that $m$ should be a multiple of $n$, or we can include all datapoints. This leads us to a "completely augmented" estimator which includes all data and all transforms (assuming $|G|$ is finite)

$$\hat{\theta}_n|G|\left(\{g_jX_i\}_{i\in[n], j\in[|G|]}\right).$$

The advantage of the above reasoning is that it allows us to design augmented/invariant learning procedures extremely generally.

3.4 Connections and perspectives

Our approach has connections to many important and well-known concepts in statistics and machine learning. Here we elaborate on those connections, which should help deepen our understanding of the problems under study.

3.4.1 Sufficiency

The notion of sufficiency, due to Ronald A. Fisher, is a fundamental concept in statistics. Given an observation (datapoint) $X$ from a statistical model $X \sim P \in \mathcal{P}$, a statistic $T := T(X)$ is said to be sufficient for a parameter $\theta := \theta(P)$ if the conditional distribution of $X|T = t$ does not depend on $\theta$ for almost any $t$. Effectively, we can reduce the data $X$ to the statistic $T$ without any loss of information about $\theta$. A statistic $T$ is said to be minimal sufficient if any other sufficient statistic is a function of it.

In our setup, assuming the invariance $X = gX$, on the invariant subspace $\Theta_G$, the orbits $G \cdot x := \{gx | g \in G\}$ are minimal sufficient for $\theta$. More generally, the local invariance condition (where invariance only holds for a subset of the parameter space) implies that the group orbits are a locally sufficient statistic for our model. From the perspective of statistical theory, this suggests that we should work with the orbits. However, this can only be practical under the following conditions:

1. We can conveniently compute the orbits, or we can conveniently find representatives
2. We can compute the distribution induced by the model on the orbits
3. We can compute estimators/learning rules defined on the orbits in a convenient way

This is possible in many cases (Lehmann and Casella, 1998; Lehmann and Romano, 2005), but in complex cases such as deep learning, some or all of these steps can be impractical. For instance, the set of transforms may include translations, rotations, scalings, shearings, color shifts, etc. How can we compute the orbit of an image? It appears that an explicit description would be hard to find.

3.4.2 Invariant representations

The notions of invariant representations and features are closely connected to our approach. Given an observation $x$, and a semi-group of transforms $G$ acting on $x \in \mathcal{X}$ by $(x, g) \rightarrow gx$, a feature $F : \mathcal{X} \rightarrow \mathcal{Y}$ is invariant if $F(x) = F(gx)$ for all $x, g$. This definition does not require a probabilistic model. By design, convolutional filters are trained to look for spatially localized features, such as edges, whose pixel-wise representation is invariant to location. In our setup, we have a group acting on the data. In that case, it is again easy to see that the orbits $G \cdot x := \{gx | g \in G\}$ are the maximal invariant representations.

Related work by Mallat, Boelcskei and others (e.g., Mallat, 2012; Bruna and Mallat, 2013; Wiatowski and Bölcskei, 2018; Anselmi et al., 2019) tries to explain how CNNs extract features, using ideas from harmonic analysis. They show that the features of certain models of neural networks (Deep Scattering Networks for Mallat) are increasingly invariant with respect to depth.
3.4.3 Equivariance

The notion of equivariance is also key in statistics (e.g., Lehmann and Casella, 1998). A statistical model is called equivariant with respect to a group $G$ acting on the sample space if there is an induced group $G^*$ acting on the parameter space $\Theta$ such that for any $X \sim P_\theta$, and any $g \in G$, there is a $g^* \in G^*$ such that $gX \sim P_{g^*\theta}$. Under equivariance, it is customary to restrict to equivariant estimators, i.e., those that satisfy $\hat{\theta}(gx) = g^*\hat{\theta}(x)$. Under some conditions, there are Uniformly Minimum Risk Equivariant (UMRE) estimators.

Our invariance condition can be viewed as having a “trivial” induced group $G^*$, which always acts as the identity. Then the equivariant estimators are those for which $\hat{\theta}(gx) = \hat{\theta}(x)$. Thus, equivariant estimators are invariant on the orbits.

The above mentioned UMRE results crucially use that the induced group has large orbits on the parameter space (or in the extreme case, is transitive), so that many parameter values are equivalent. In contrast, we have the complete opposite setting, where the orbits are singletons. Thus our setting is very different from classical equivariance.

3.4.4 Variance reduction in Monte Carlo

Variance reduction techniques are widely used in Monte Carlo methods (Robert and Casella, 2013). Data augmentation can be viewed as a type of variance reduction, and is connected to other known techniques. For instance, $f(gX)$ can be viewed as control variates for the random variable $f(X)$. The reason is that $f(gX)$ has the same marginal distribution, and hence the same mean as $f(X)$. Taking averages can be viewed as a suboptimal, but universal way to combine control variates.

We briefly mention that under a reflection symmetry assumption, data augmentation can also be viewed as a special case of the method of antithetic variates.

3.4.5 Connection to data augmentation

We can summarize the connections to the areas mentioned above. Data augmentation is computationally feasible approach to approximately learn on the orbits (which are both the minimal sufficient statistics and maximal invariant features).

The computational efficiency is partly because we never explicitly compute or store the orbits and invariant features. However, in deep learning, the outputs of the layers deep into the architecture are approximations to the invariant features, at least those that are relevant to the learning problem (e.g., classification) at hand.

4 Theoretical results

In this section, we present our theoretical results for data augmentation, starting with some general results on variance reduction.

4.1 General estimators

To study the variance reduction due to data augmentation, we present an invariance lemma that characterizes the bias and variance of estimators under augmentation.

Lemma 4.1 (Invariance lemma). Let $f$ be an arbitrary function with finite variance under $P$, and assume we have a distribution $X \sim P$ such that $X =_d gX$ for all $g \in G$. Consider an arbitrary distribution $\mu$ on $G$. Let $\overline{f}(x) = \mathbb{E}_\mu f(gx)$, where $g \sim \mu$. Then:

1. $\overline{f}(X)$ is (a version of the) the conditional expectation of the random variable $f(X)$, conditional on the orbit $X \in G \cdot x$.
2. Therefore, the mean of $\overline{f}(X)$ and $f(X)$ coincide: $\mathbb{E}_P f(X) = \mathbb{E}_P \overline{f}(X)$. 

3. The two covariance matrices of the random variables $f(X)$ and $f(gX)$, where $g$ is distributed according to $\mu$, are equal: $\text{Cov}_Pf(X) = \text{Cov}_{P,\mu}f(gX)$.

4. Hence, the law of the “total covariance” implies that the covariance of $f(X)$ is the sum of the covariance of the conditional mean on orbits, and the average covariance within orbits:

$$\text{Cov}_Pf(X) = \text{Cov}_Pf(X) + \mathbb{E}_{P}\text{Cov}_{\mu}f(gX).$$

5. Let us define the covariance of $f$ with its copy shifted by $g$: $C(f;h) = \text{Cov}_P[f(X), f(hX)^\top]$. We can then express the covariance of the mean as the average of shifted covariances, as well as the covariance of $f$ with its mean.

$$\text{Cov}_P\overline{f}(X) = \mathbb{E}_{\mu\sim\mu} C(f; h) = \text{Cov}_P[f(X), \overline{f}(X)].$$

See Figure 3 for an illustration of orbit averaging.

Proof. These results follow from simple calculation:

1. This is true by inspection.

2. This follows from the above point. Alternatively, we can verify directly that we have

$$\mathbb{E}_P\overline{f}(X) = \mathbb{E}_P\mathbb{E}_\mu f(gX) = \mathbb{E}_\mu \mathbb{E}_P f(gX) = \mathbb{E}_\mu \mathbb{E}_P f(X) = \mathbb{E}_P f(X).$$

The key property that we used is that $\mathbb{E}_P f(gX) = \mathbb{E}_P f(X)$ for any $g$.

3. First, we have for any fixed $g \in G$ that $\text{Cov}_P f(X) = \text{Cov}_P f(gX)$. Since the right hand side does not depend on $g$, we can take an average over $\mu$, and we obtain the desired result.

4. This property follows directly from the law of the total covariance applied to the random variable $f(gX)$, where $g \sim \mu$. Alternatively, we can derive it using a direct calculation as follows. We have

$$\text{Cov}_P f(X) = \mathbb{E}_P f(X)f(X)^\top + \mathbb{E}_P f(X)\mathbb{E}_P f(X)^\top$$

$$\text{Cov}_P \overline{f}(X) = \mathbb{E}_P \overline{f}(X)\overline{f}(X)^\top + \mathbb{E}_P \overline{f}(X)\mathbb{E}_P \overline{f}(X)^\top$$

From the first part, the second terms on the right hand side are equal to each other. Therefore, we only need to evaluate

$$\mathbb{E}_P f(X)f(X)^\top - \mathbb{E}_P \overline{f}(X)\overline{f}(X)^\top = \mathbb{E}_P \mathbb{E}_\mu f(gX)f(gX)^\top - \mathbb{E}_P [\mathbb{E}_\mu f(gX)\mathbb{E}_\mu f(gX)^\top]$$

$$= \mathbb{E}_P [\mathbb{E}_\mu f(gX)f(gX)^\top - \mathbb{E}_\mu f(gX)\mathbb{E}_\mu f(gX)^\top]$$

$$= \mathbb{E}_P \text{Cov}_\mu f(gX)$$

as desired. In the first line we used $\mathbb{E}_P f(X)f(X)^\top = \mathbb{E}_P \mathbb{E}_\mu f(gX)f(gX)^\top$, which is a consequence of the previous results for the function $f(X)f(X)^\top$. 

Figure 3: Orbit averaging
5. We can assume without loss of generality that $f$ has mean zero under $\mathbb{P}$. We can then write
\[
\text{Cov}_\mathbb{P} \overline{f}(X) = \mathbb{E}_\mathbb{P} \mathbb{E}_{g \sim \mu} f(gX) \mathbb{E}_{g' \sim \mu} f(g'X)^	op
\]
\[
= \mathbb{E}_{g, g' \sim \mu} \mathbb{E}_\mathbb{P} f(gX) f(g'X)^	op
\]
\[
= \mathbb{E}_{g, g' \sim \mu} \mathbb{E}_\mathbb{P} f(X) f(g' : g^{-1}X)^	op
\]
\[
= \mathbb{E}_{h \sim \mu} \mathbb{E}_\mathbb{P} f(X) f(hX)^	op
\]
\[
= \mathbb{E}_{h \sim \mu} C(f; h)
\]
\[
= \text{Cov}_\mathbb{P} [f(X), \overline{f}(X)].
\]

\[\square\]

**Augmentation leads to variance reduction.** This simple lemma immediately implies that data augmentation has favorable variance reduction properties. For general estimators, we obtain a direct consequence:

**Proposition 4.2** (Augmentation decreases MSE of general estimators). Consider an estimator $\hat{\theta}(x)$ of $\theta$, and its augmented version $\hat{\theta}_A(x) = \mathbb{E}_G \hat{\theta}(gx)$. The bias of the augmented estimator is the same as the bias of the original estimator, and the covariance matrix of the augmented estimator becomes smaller than or equal to in the Loewner order:

\[
\text{Cov} [\hat{\theta}_A(x)] \preceq \text{Cov} [\hat{\theta}(x)].
\]

Hence, the MSE decreases by augmentation.

For other estimators based on the augmentation distribution, such as the median, one can show that other measures of error, such as the mean absolute error decrease. For ERM and MLE, the claim implies that the the variance of the augmented loss, log-likelihood, and score functions all decreases. This shows how data augmentation can be viewed as a form of algorithmic regularization. Indeed, the mean behavior of loss/log-likelihood, etc are all unchanged, but the variance decreases. This indeed shows that augmentation is a natural form of regularization.

**Technical details.** As a technical detail, we present a finer analysis of “orbit averaging” and “conditioning on orbits”. We have stated in the invariance lemma that $\mathbb{E}_{g \sim \mu} f(gX)$ is a version of $\mathbb{E}_X [f(X) | X \in GX]$ under very general conditions. We need a few extra regularity conditions for this to hold, as explained in the following lemma.

**Lemma 4.3.** Let $X \sim \mathbb{P}$. Assume that for all $g$ in the group $G$, we have $X =_d gX$. Let $\mathbb{Q}$ be the Haar measure on $G$. Let $f$ be an arbitrary function so that $(X, g) \mapsto f(gX)$ is in $L^1(\mathbb{P} \times \mathbb{Q})$. Define $\overline{f}(x) = \mathbb{E}_G f(gx)$. Then:

1. $\overline{f}(X) = \mathbb{E}_\mathbb{P} [f(X) | X \in GX] \ \mathbb{P}\text{-a.s, where } GX = \{gX : g \in G\}$;
2. Let $\varphi$ be any real-valued convex function. Then $\mathbb{E}_\mathbb{P} [\varphi(f(X))] \geq \mathbb{E}_\mathbb{P} [\varphi(\overline{f}(X))]$.

**Proof.** To check the first claim, note that $\overline{f}(X) = \int f(gX) d\mathbb{Q}(g)$, and $\mathbb{Q}$ is Haar, so knowing the orbit allows one to explicitly compute the integral, which means $\overline{f}(X)$ is indeed measurable w.r.t. $\sigma(GX)$, the $\sigma$-field generated by the orbit. Then taking any event $A \in \sigma(GX)$, we have
\[
\int_{X \in A} \int_G f(gX) d\mathbb{Q}(g) d\mathbb{P}(X) = \int_G \int_X f(gX) 1\{X \in A\} d\mathbb{P}(X) d\mathbb{Q}(g)
\]
\[
= \int_G \int_X f(gX) 1\{gX \in gA\} d\mathbb{P}(X) d\mathbb{Q}(g)
\]
\[
= \int_G \int_X f(X) 1\{X \in gA\} d\mathbb{P}(X) d\mathbb{Q}(g)
\]
\[
= \int_G \int_X f(X) 1\{X \in A\} d\mathbb{P}(X) d\mathbb{Q}(g)
\]
\[
= \int_X f(X) 1\{X \in A\} d\mathbb{P}(X),
\]

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where in the first line we used Fubini’s theorem, in the third line we used $X =_d gX$, and in the fourth line we used $A \in \sigma(GX)$. Then by definition of conditional expectation, we have proved the first claim. Finally, by Jensen’s inequality, we have

$$
\mathbb{E}_g[\varphi(f(X)) \mid X \in GX] \geq \varphi(\mathbb{E}_g[f(X) \mid X \in GX]) = \varphi(\mathbb{E}(X)).
$$

Then taking the expectation w.r.t. $\mathbb{E}_g$ gives the second claim.

If an estimator $\hat{\theta}(X)$ satisfies the conditions in the above lemma, we then know that for any convex loss function $L(\theta_0, \cdot)$ (where $\theta_0$ is the true parameter), we have

$$
\mathbb{E}_L(\theta_0, \hat{\theta}(X)) \geq \mathbb{E}_L(\theta_0, \mathbb{E}_G(\hat{\theta}(gX)).
$$

So we see that the augmented estimator $\mathbb{E}_G(\hat{\theta}(gX)$ is no worse than the original estimator.

An important question now is that how much do we gain by the orbit averaging operation. Note that this question is in the same fashion of asking “how much do we gain by Rao-Blackwellizing an estimator”. Inspecting the proof of the previous lemma, we see that this question is equivalent to characterizing the “Jensen gap”:

$$
\mathbb{E}_L[\varphi(f(X)) \mid X \in GX] - \varphi(\mathbb{E}_L[f(X) \mid X \in GX]).
$$

There are some results on lower bounding the Jensen gap under such full generality (see, e.g., Liao and Berg 2018 and references therein). To fully characterize the gap, it is necessary to do a case-by-case analysis. We provide a well-known example from classical statistics:

**Example 4.4** (U-statistic as an augmented estimator). Consider data $X_1, \ldots, X_n$ iid from some distribution $\mathbb{P}$. We are interested in estimating some functional $\theta$ of $\mathbb{P}$. Suppose we have a crude preliminary estimator $\theta(X_1, \ldots, X_r)$, which takes $r < n$ arguments and is permutation-invariant on its arguments. Let $G$ be the permutation group acting on $(X_1, \ldots, X_n)$. Then the augmented estimator is

$$
\mathbb{E}_G[\hat{\theta}(gX_1, \ldots, X_n)] = \frac{1}{\binom{n}{r}} \sum_{i_1 < i_2 < \cdots < i_r} \hat{\theta}(X_{i_1}, \ldots, X_{i_r}).
$$

This is the U-statistic of order $r$ with kernel $\hat{\theta}$. It is known that the statistical properties of the U-statistic are far better than its non-augmented counterpart, which does not use all the data. There are well-known explicit formulas for the variance reduction (e.g., Van der Vaart, 1998).

**Beyond groups.** Some of our conclusions hold without requiring a group structure on the set of transforms. Instead, it is enough to consider a set (i.e., a semigroup, because the identity always makes sense to include) of transforms $T : \mathbb{R}^d \to \mathbb{R}^d$, with a probability measure $\mu$ on them. This is more realistic in some applications, e.g., in deep learning where we also consider transforms such as cropping images, which are not invertible. Then we still get the variance reduction in Lemma 4.1. Therefore, under appropriate regularity conditions, we also get the improvement in the performance of augmented ERM, as stated previously, as well as in the next sections. However, some of the results and interpretations do not hold in this more general setting. Specifically, the orbits are not necessarily defined anymore, and so we cannot view the augmented estimators as conditional expectations over orbits.

### 4.2 ERM / M-estimators

#### 4.2.1 Non-asymptotic results

We now move on to present our results on the behavior of ERM. Using the prior results on variance reduction, we can show quite directly, based on results from stochastic convex optimization, that augmentation reduces the variance of the learned parameters. Suppose the loss function $\theta \to L(\theta, x)$ is strongly convex with respect to $\theta$, for any $x$, with a strong convexity constant $\lambda > 0$. Assume $L$ is differentiable with respect to $\theta$ and let $\sigma^2 = \text{Var}_X[\nabla_\theta L(\theta, X)]$ be the variance of the gradient (i.e., the trace of the covariance matrix $\text{Cov}[\nabla_\theta L(\theta, X)]$). Let $\theta^*$ be the minimizer of the population risk $\mathbb{E}_X \sim P L(\theta, X)$.
Then there are several results in stochastic convex optimization and statistical learning about the convergence rate of $\hat{\theta}_L$. We choose to use a particularly simple and elegant result from Foster et al. (2019) (see their Theorem 7). This shows that any minimizer $\tilde{\theta}_L$ of the empirical risk (1) has mean squared error
\[
\E \|\tilde{\theta}_L - \theta^*\|^2 \leq \frac{4\sigma^2}{\lambda^2 n}.
\]

Data augmentation reduces the variance:

**Proposition 4.5** (Data augmentation reduces variance in ERM). Let $\tilde{\sigma}^2 = \text{Var}_X[\nabla \tilde{L}(\theta, X)]$ be the variance of the gradient of the augmented loss function. Any minimizer $\hat{\theta}_L$ of the augmented empirical risk (3) has mean squared error
\[
\E \|\hat{\theta}_L - \theta^*\|^2 \leq \frac{4\tilde{\sigma}^2}{\lambda^2 n}.
\]

Moreover, $\tilde{\sigma}^2 \leq \sigma^2$, so this bound is sharper than for ERM.

**Proof.** The proof is simply a matter of checking the conditions required by Foster et al. (2019). It is not hard to see that the strong convexity is preserved under averaging, and so the strong convexity constant of $\theta \to \tilde{L}(\theta, x) = \E_{g \sim Q} L(\theta, gx)$ is at least as large as that of $\theta \to L(\theta, x)$. Moreover, using the law of total variance, it is similar not hard to see that $\tilde{\sigma}^2 \leq \sigma^2$.

The above result shows that we get a sharper upper bound on the MSE. However, this is somewhat unsatisfactory, because it is only an upper bound, and thus it does not precisely tell us how much we gain. To see this more clearly, we will later adopt an asymptotic approach.

### 4.2.2 Generalization bound via Rademacher complexity

In this section, we show how to obtain a non-asymptotic generalization bound via Rademacher complexity (Bartlett and Mendelson, 2002). For consistency with the rest of the paper, we will adopt the parametric model, though it is possible to derive similar results under a more general PAC learning framework. Let $\theta$ be a minimizer of the population risk. We want to show that $\theta$ generalizes on unseen data. That is, we want to give a high probability upper bound on the following generalization gap:
\[
\E L(\hat{\theta}, X) - \E L(\theta_0, X).
\]

Notice that $\E L(\hat{\theta}, X)$ means evaluating the function $\theta \mapsto \E L(\theta, X)$ at the random point $\theta = \hat{\theta}$, and is hence random.

From a high level, there are two common approaches to prove such a bound. The first one is *algorithm-independent* and usually based on some Glivenko-Cantelli type uniform convergence results. The second one is *algorithm-dependent* and usually relies on some notions of stability of the learning algorithm (e.g., stochastic gradient descent) (see e.g., Shalev-Shwartz and Ben-David, 2014). Since our paper focuses on demonstrating the performance of the augmented loss function, we will develop algorithm-independent bounds, though algorithm-dependent bounds may be derived using similar techniques.

First we recall the known proof providing bounds on the generalization bounds via Rademacher complexity. We present this only for pedagogical reasons, as a warmup for the following part on data augmentation.

We start with the natural decomposition:
\[
\E L(\tilde{\theta}, X) - \E L(\theta_0, X) = \E L(\tilde{\theta}, X) - \frac{1}{n} \sum_{i=1}^n L(\tilde{\theta}, X_i) + \frac{1}{n} \sum_{i=1}^n L(\tilde{\theta}, X_i) - \E L(\theta_0, X).
\]

The second half of the RHS above can be decomposed as
\[
\frac{1}{n} \sum_{i=1}^n L(\tilde{\theta}, X_i) - \E L(\theta_0, X) = \frac{1}{n} \sum_{i=1}^n L(\tilde{\theta}, X_i) - \frac{1}{n} \sum_{i=1}^n L(\tilde{\theta}, X_i) + \frac{1}{n} \sum_{i=1}^n L(\theta_0, X_i) - \E L(\theta_0, X)
\]
\[
\leq \frac{1}{n} \sum_{i=1}^n L(\theta_0, X_i) - \E L(\theta_0, X),
\]

where the inequality holds because \( \hat{\theta} \) is a minimizer of the empirical risk. Hence we arrive at

\[
\mathbb{E} L(\hat{\theta}, X) - \mathbb{E} L(\theta_0, X) \leq \frac{1}{n} \sum_{i=1}^{n} L(\hat{\theta}, X_i) + \frac{1}{n} \sum_{i=1}^{n} L(\theta_0, X_i) - \mathbb{E} L(\theta_0, X)
\]

\[
\leq \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| + \left( \frac{1}{n} \sum_{i=1}^{n} L(\theta_0, X_i) - \mathbb{E} L(\theta_0, X) \right).
\]

By McDiarmid’s inequality, we have

\[
\mathbb{P}\left( \frac{1}{n} \sum_{i=1}^{n} L(\theta_0, X_i) - \mathbb{E} L(\theta_0, X) > t \right) \leq \exp\{-2nt^2\}.
\]

So w.p. at least \( 1 - \delta/2 \), we have

\[
\frac{1}{n} \sum_{i=1}^{n} L(\theta_0, X_i) - \mathbb{E} L(\theta_0, X) \leq \sqrt{\frac{\log 2/\delta}{2n}}.
\]

It remains to control

\[
\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right|.
\]

We bound the above quantity using Rademacher complexity. The arguments are standard and can be found in many textbooks (see, e.g., Shalev-Shwartz and Ben-David 2014). For simplicity, we will assume the loss function \( L(\theta, x) \in [0, 1] \) for any \( \theta \) and \( x \). For two data sets \( \{X_i\}_i^n \) and \( \{\tilde{X}_i\}_i^n \) which only differ in the \( i \)-th coordinate, we have

\[
\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| - \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, \tilde{X}_i) - \mathbb{E} L(\theta, X) \right| \leq \frac{1}{n} \sup_{\theta \in \Theta} |L(\theta, X_i) - L(\theta, \tilde{X}_i)| \leq \frac{1}{n}.
\]

By McDiarmid’s inequality, we have

\[
\mathbb{P}\left( \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| - \mathbb{E} \left[ \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| \right] \geq t \right) \leq \exp\{-2nt^2\}.
\]

It follows that w.p. \( 1 - \delta/2 \), we have

\[
\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| - \mathbb{E} \left[ \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| \right] \leq \sqrt{\frac{\log 2/\delta}{2n}}.
\]

A standard symmetrization argument then shows that

\[
\mathbb{E} \left[ \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) - \mathbb{E} L(\theta, X) \right| \right] \leq 2R_n(L \circ \Theta),
\]

where the Rademacher complexity of the function class \( L \circ \Theta = \{x \mapsto L(\theta, x) : \theta \in \Theta\} \) is defined as

\[
R_n(L \circ \Theta) = \mathbb{E} \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} \varepsilon_i L(\theta, X_i) \right|,
\]

where the expectation is taken over both the data and IID Rademacher random variables \( \varepsilon_i \), which are independent of the data. Summarizing the above computations (along with a union bound), we arrive at the following classical proposition.

**Proposition 4.1** (Classical Rademacher generalization bound). *With probability at least 1 - \( \delta \), we have

\[
\mathbb{E} L(\hat{\theta}, X) - \mathbb{E} L(\theta_0, X) \leq 2R_n(L \circ \Theta) + \sqrt{\frac{2 \log 2/\delta}{n}}.
\]
This generalization bound is a standard result. It can be viewed as an intermediate between Theorems 26.3 and Theorem 26.5 of Shalev-Shwartz and Ben-David (2014), part 3, because it is a high-probability bound (like 26.5) for expected generalization error (like 26.3).

We now consider the augmented ERM. In this section, we do not require $g_X = d X$. Let $\hat{\theta}_G$ minimize the augmented loss $\sum_{i=1}^n E_G L(\theta, gX_i)/n$. We start by doing a similar decomposition

$$ EL(\hat{\theta}_G, X) - EL(\theta_0, X) = I + II + III + IV + V, $$

where

$$ I = EL(\hat{\theta}_G, X) - E \sum_i^n E_G L(\hat{\theta}_G, gX_i) $$

$$ II = E \sum_i^n E_G L(\hat{\theta}_G, gX_i) - \frac{1}{n} \sum_i^n E_G L(\theta_0, gX_i) $$

$$ III = \frac{1}{n} \sum_i^n E_G L(\hat{\theta}_G, gX_i) - \frac{1}{n} \sum_i^n E_G L(\theta_0, gX_i) $$

$$ IV = \frac{1}{n} \sum_i^n E_G L(\theta_0, gX_i) - E \sum_i^n E_G L(\theta_0, gX_i) $$

$$ V = E \sum_i^n E_G L(\theta_0, gX) - EL(\theta_0, X). $$

By construction, we have $III \leq 0$ and $II + IV \leq 2 sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_G L(\theta, gX_i) - E \sum_i^n E_G L(\theta, gX_i) \right|.$

Moreover, we have $I + V \leq 2 sup_{\theta \in \Theta} \left| EL(\theta, X) - E \sum_i^n E_G L(\theta, gX_i) \right|,$

which is equal to zero under exact invariance $gX = d X$. The plan is to bound $II + IV$ using Rademacher complexity and to bound $I + V$ via the Wasserstein-1 distance between $X$ and $gX$. We now bound $II + IV$. An application of McDiarmid’s inequality with a symmetrization argument gives

$$ II + IV \leq 2 \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_G L(\theta, gX_i) - E \sum_i^n E_G L(\theta, gX_i) \right| + \sqrt{\frac{2 \log 2/\delta}{n}}. $$

w.p. at least $1 - \delta$, where

$$ R_n(L_G \circ \Theta) = \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_G L(\theta, gX_i) \right| $$

$$ \leq \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_G L(\theta, gX_i) \right| $$

$$ = E_G \left[ \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_i L(\theta, gX_i) - E \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_i^n E_i L(\theta, X_i) \right| \right] + R_n(L \circ \Theta). $$

We now assume the our loss function is uniformly Lipschitz on the data w.r.t. some lower semi-continuous metric $d(\cdot, \cdot)$ on the sample space $X$ (where $X$ takes values on). That is, for any $x, \bar{x} \in X$, $\theta \in \Theta$, we have

$$ L(\theta, x) - L(\theta, \bar{x}) \leq ||L||_{\text{Lip}} \cdot d(x, \bar{x}) $$

for some constant $||L||_{\text{Lip}}$. For a fixed vector $(\varepsilon_1, \ldots, \varepsilon_n)$, consider the function

$$ h : (x_1, \ldots, x_n) \mapsto \sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^n \varepsilon_i L(\theta, x_i) \right|. $$
We have
\[ |h(x_1, \ldots, x_n) - h(y_1, \ldots, y_n)| \leq \frac{1}{n} \sup_{\theta \in \Theta} \left| \sum_{i=1}^{n} \varepsilon_i L(\theta, x_i) - \varepsilon_i L(\theta, y_i) \right| \]
\[ \leq \frac{1}{n} \|L\|_{\text{Lip}} \cdot \sum_i d(x_i, y_i). \]

That is, the function \( h : \mathcal{X}^n \to \mathbb{R} \) is \( (\|L\|_{\text{Lip}}/n) \)-Lipschitz w.r.t. the l.s.c. metric \( d_n \), defined by \( d_n(\{x_i\}_1^n, \{y_i\}_1^n) = \sum_i d(x_i, y_i) \). We now recall the definition of the Wasserstein-1 distance.

**Definition 4.6.** Let \( \mathcal{X} \) be a Polish space. Let \( d \) be a lower semi-continuous (l.s.c) metric on \( \mathcal{X} \). For two probability distributions \( \mu, \nu \) on \( \mathcal{X} \), we define
\[ W_d(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{X}} d(x, y) d\pi(x, y), \]
where \( \Pi(\mu, \nu) \) are all couplings whose marginals agree with \( \mu \) and \( \nu \).

We will need the following lemma, which is a triangle inequality for Wasserstein-1 distance. We remark that that the same inequality for total variation distance is more well-known, and the proofs are essentially identical.

**Lemma 4.7** (Triangle inequality/Tensorization). For two random vectors \((X_1, \ldots, X_n), (Y_1, \ldots, Y_n) \in \mathcal{X}^n\), we denote the joint laws as \( \mu^n, \nu^n \) respectively, and the marginal laws as \( \{\mu_i\}_1^n, \{\nu_i\}_1^n \) respectively. We have
\[ W_d(\mu^n, \nu^n) \leq \sum_i W_d(\mu_i, \nu_i). \]

**Proof.** By Kantorovich duality (see, e.g., Villani 2003), for each coordinate, we can choose optimal couplings \((X^*_i, Y^*_i) \in \Pi(\mu_i, \nu_i)\) s.t. \( W_d(X_i, Y_i) = Ed(X^*_i, Y^*_i) \). We then conclude that proof by noting that \((\{X^*_i\}_1^n, \{Y^*_i\}_1^n) \in \Pi(\mu^n, \nu^n)\).

Applying the Kantorovich-Rubinstein theorem, i.e., the dual representation of the Wasserstein metric (see, e.g., Villani 2003), for arbitrary random vectors \((X_1, \ldots, X_n)\) and \((Y_1, \ldots, Y_n)\), we have
\[ |Ed(X_1, \ldots, X_n) - h(Y_1, \ldots, Y_n)| \leq \frac{1}{n} \|L\|_{\text{Lip}} \cdot W_d(\mu^n, \nu^n) \leq \frac{1}{n} \|L\|_{\text{Lip}} \cdot \sum_{i=1}^{n} W_d(X_i, Y_i). \]

Hence we arrive at
\[ R_n(L_G \circ \Theta) \leq R_n(L \circ \Theta) + \|L\|_{\text{Lip}} \cdot \frac{1}{n} \sum_i \mathbb{E}_G W_d(X_i, gX_i) = R_n(L \circ \Theta) + \|L\|_{\text{Lip}} \cdot \mathbb{E}_G W_d(X, gX). \]

Summarizing the above computations, we have
\[ II + IV \leq 2R_n(L \circ \Theta) + \|L\|_{\text{Lip}} \cdot \mathbb{E}_G W_d(X, gX) + \sqrt{\frac{2 \log 2/\delta}{n}} \]
w.p. at least \( 1 - \delta \). We now bound \( I + V \). We have
\[ I + V \leq 2 \sup_{\theta \in \Theta} \left| EL(\theta, X) - \mathbb{E}_G L(\theta, gX) \right| \]
\[ \leq 2 \sup_{\theta \in \Theta} \left| EL(\theta, X) - EL(\theta, gX) \right| \]
\[ \leq 2 \|L\|_{\text{Lip}} \cdot W_d(X, gX). \]

We collect the above results into a proposition.
Proposition 4.2 (Rademacher generalization bound for data augmentation). Let $L(\theta, \cdot)$ be Lipschitz w.r.t. some lower semi-continuous metric $d$ on the sample space $\mathcal{X}$, uniformly over $\theta \in \Theta$. Assume that the loss is bounded in the unit interval, $L(\cdot, \cdot) \in [0, 1]$. Let $\theta, \theta_G$ be minimizers of the empirical risk and the augmented empirical risk, respectively. Let $\theta_0$ be a minimizer of the population risk. Then with probability at least $1 - \delta$ over the draw of $X_1, \ldots, X_n$, we have

$$\mathbb{E}L(\hat{\theta}, X) - \mathbb{E}L(\theta_0, X) \leq 2\mathcal{R}_n(L \circ \Theta) + \sqrt{\frac{2 \log 2/\delta}{n}}$$

$$\mathbb{E}L(\hat{\theta}_G, X) - \mathbb{E}L(\theta_0, X) \leq 2\mathcal{R}_n(L_G \circ \Theta) + \sqrt{\frac{2 \log 2/\delta}{n}} + 2\|L\|_{\text{Lip}} \cdot \mathbb{E}W_d(X, gX),$$

where the Rademacher complexity $\mathcal{R}_n(L_G \circ \Theta)$ of the augmented loss class can further be bounded as

$$\mathcal{R}_n(L_G \circ \Theta) \leq \mathcal{R}_n(L \circ \Theta) + \|L\|_{\text{Lip}} \cdot \mathbb{E}W_d(X, gX).$$

In particular, if $X =_d gX$, then $\mathcal{R}_n(L_G \circ \Theta) \leq \mathcal{R}_n(L \circ \Theta)$, so augmentation decreases the Rademacher complexity.

Similarly to before, this shows that we can get a sharper upper bound for the augmented ERM. However, it still does not tell us precisely how much we gain, as it is only an upper bound. This motivates us to consider asymptotics.

4.2.3 Asymptotics of ERM / M-estimators

We now move to asymptotics for ERM/M-estimation. Consider $\mathbb{R}^d$-valued data $X_1, \ldots, X_n \overset{iid}{\sim} \mathbb{P}$ with density $f$. We are interested in estimating a parameter $\theta$ attached to the data-generating distribution $\mathbb{P}$. Consider a criterion function $L(\theta, \cdot) : \mathbb{R}^d \to \mathbb{R}$, so that the true parameter $\theta_0$ is a minimizer of $\mathbb{E}L(\theta, X)$, where $X \sim \mathbb{P}$ over a parameter space $\theta \in \Theta \subseteq \mathbb{R}^p$. In order to estimate $\theta_0$, we (approximately) minimize the random function:

$$\min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n L(\theta, X_i).$$

In the classical regime where $p$ is fixed and $n \to \infty$, we have the following two well-known results. We denote by $\overset{p}{\to}$ convergence in probability, and by $o_p(1)$ a term that converges in probability to zero.

Theorem 4.8 (Van der Vaart 1998, Theorem 5.21). Assume that for every $\varepsilon > 0$, we have

$$\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^n L(\theta, X_i) - \mathbb{E}L(\theta, X) \right| \overset{p}{\to} 0,$$

$$\sup_{\theta : \|\theta - \theta_0\| \geq \varepsilon} \mathbb{E}L(\theta, x) > \mathbb{E}L(\theta_0, x).$$

Then any sequence of estimators $\hat{\theta}_n$ with

$$\frac{1}{n} \sum_{i=1}^n L(\hat{\theta}_n, X_i) \leq \frac{1}{n} \sum_{i=1}^n L(\theta_0, X_i) + o_p(1)$$

converges in probability to $\theta_0$.

Theorem 4.9 (Van der Vaart 1998, Theorem 5.23). Assume $\Theta$ is open. For each $\theta \in \Theta$, let $x \mapsto L(\theta, x)$ be measurable and let $\theta \mapsto L(\theta, x)$ be differentiable at $\theta_0$ on a set of $x$ with full measure with respect to $\mathbb{P}$, with derivative $\nabla L(\theta_0, x)$. Assume that there exists a $L^2(\mathbb{P})$ function $\tilde{L}$ such that for every $\theta_1, \theta_2$ in a neighborhood of $\theta_0$, we have

$$|L(\theta_1, x) - L(\theta_2, x)| \leq \tilde{L}(x)\|\theta_1 - \theta_2\|.$$
Furthermore, assume that the map \( \theta \mapsto \mathbb{E}L(\theta, X) \) admits a second-order Taylor expansion at \( \theta_0 \) with non-singular symmetric second derivative matrix \( V_{\theta_0} \). If \( \hat{\theta}_n \) is an approximate minimizer:
\[
\frac{1}{n} \sum_{i=1}^{n} L(\hat{\theta}_n, X_i) \leq \inf_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} L(\theta, X_i) + o_p(n^{-1}),
\]
and \( \hat{\theta}_n \to \theta_0 \), then \( \hat{\theta}_n \) has the following Bahadur representation
\[
\sqrt{n}(\hat{\theta}_n - \theta_0) = \frac{1}{\sqrt{n}} V_{\theta_0}^{-1} \sum_{i=1}^{n} \nabla L(\theta_0, X_i) + o_p(1).
\]
In particular,
\[
\sqrt{n}(\hat{\theta}_n - \theta_0) \Rightarrow N(0, V_{\theta_0}^{-1} \mathbb{E}[\nabla L(\theta_0, \cdot) \nabla L(\theta_0, \cdot)'] | V_{\theta_0}^{-1}).
\]

**Symmetry.** Suppose now we have additional symmetry structure. We assume there is a group \( G \) which acts linearly on \( \mathbb{R}^d \), and that for \( X \sim \mathbb{P}, g \in G \), we have
\[
gX = d \ X.
\]
The assumption above says that
\[
f(g^{-1}x)/ \det g = f(x) \ \mathbb{P}\text{-a.s. } x.
\]
Note that when \( G \) acts orthogonally on \( \mathbb{R}^p \), we have \( \det g = 1 \) and thus the invariance reads:
\[
f(gx) = f(x).
\]

We assume the group \( G \) is endowed with its Haar measure \( \mathbb{Q} \). We denote the expectation w.r.t. \( \mathbb{Q} \) as \( \mathbb{E}_G \). As discussed above, we consider the natural criterion function \( \mathbb{E}_GL(\theta, gx) \), and we consider the natural estimator
\[
\min_{\theta \in \Theta} \sum_{i=1}^{n} \mathbb{E}_GL(\theta, gX_i).
\]

**Lemma 4.10.** Assume \( \Theta \) is open. For each \( \theta \in \Theta \), assume that the map \((g, X) \mapsto L(\theta, gX)\) is in \( L^1(\mathbb{P} \times \mathbb{Q}) \). If \( \theta_0 \in \arg \min_{\theta \in \Theta} \mathbb{E}_GL(\theta, X) \) , then
\[
\theta_0 \in \arg \min_{\theta \in \Theta} \mathbb{E}_GL(\theta, gX).
\]

**Proof.** Under the current assumption, Fubini’s theorem applies and we have \( \mathbb{E}_GL(\theta, gX) = \mathbb{E}_CL(\theta, gX) \). Note that \( gX = d X \) for a fixed \( g \) , which gives \( \mathbb{E}L(\theta, gX) = \mathbb{E}L(\theta, X) \). Hence we have \( \mathbb{E}_GL(\theta, gX) = \mathbb{E}L(\theta, gX) \), which is sufficient for the desired result. \( \square \)

We then show that the augmented estimator with the new criterion function is consistent, provided the original estimator satisfies the conditions in Theorem 4.8, plus some very weak extra assumptions.

**Proposition 4.3** (Consistency of augmented estimator). Assume the conditions in Lemma 4.10 and Theorem 4.8. Then any sequence of estimators \( \hat{\theta}_{n,G} \) with
\[
\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_GL(\hat{\theta}_{n,G}, gX_i) \leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_GL(\theta_0, gX_i) + o_p(1)
\]
converges in probability to \( \theta_0 \).
**Proposition 4.4** (Augmentation improves ERM).

Assuming the consistency of the augmented estimator, the augmented one is consistent via Theorem 4.8. Assuming the consistency of the augmented estimator, the next proposition shows that if the original estimator is asymptotically normal via Theorem 4.9, then the augmented one also asymptotically normal, but with smaller asymptotic variance.

**Proof.** We verify the two conditions required by Theorem 4.8. We have

\[
\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^{n} E_G L(\theta, gX_i) - E E_G L(\theta, gX) \right| = \sup_{\theta \in \Theta} \left| E_G \left\{ \frac{1}{n} \sum_{i=1}^{n} L(\theta, gX_i) - EL(\theta, gX) \right\} \right|
\]

\[
\leq \sup_{\theta \in \Theta} E_G \left\{ \frac{1}{n} \sum_{i=1}^{n} L(\theta, gX_i) - EL(\theta, gX) \right\}
\]

\[
\leq E_G \sup_{\theta \in \Theta} \left\{ \frac{1}{n} \sum_{i=1}^{n} L(\theta, gX_i) - EL(\theta, gX) \right\}
\]

\[
= E_G [o_p(1)]
\]

where the last inequality is because \( gX \equiv d X \). On the other hand, we check that

\[
\sup_{\theta : \|\theta - \theta_0\| \geq \varepsilon} E E_G L(\theta, gX) = \sup_{\theta : \|\theta - \theta_0\| \geq \varepsilon} E G L(\theta, gX)
\]

\[
= \sup_{\theta : \|\theta - \theta_0\| \geq \varepsilon} E L(\theta, X)
\]

\[
> E L(\theta_0, X).
\]

Hence invoking Theorem 4.8 gives the desired result. \(\Box\)

From a high level, the above proposition says that the augmented estimator is consistent, provided the original one is consistent via Theorem 4.8. Assuming the consistency of the augmented estimator, the next proposition shows that if the original estimator is asymptotically normal via Theorem 4.9, then the augmented one also asymptotically normal, but with smaller asymptotic variance.

**Proposition 4.4** (Augmentation improves ERM). Assume the same conditions as in Lemma 4.10 and Theorem 4.9. Then we have:

1. the map \( \theta \mapsto E_G L(\theta, gx) \) is differentiable at \( \theta_0 \) in \( P \)-probability;
2. the function \( E_G L(gx) \) is in \( L^2(\mathbb{P}) \) and \( |E_G L(\theta_1, gx) - E_G L(\theta_2, gx)| \leq E_G L(gx) \|\theta_1 - \theta_2\| \) for every \( \theta_1, \theta_2 \) in a neighborhood of \( \theta_0 \);
3. the map \( \theta \mapsto E E_G L(\theta, gX) \) admits a second-order Taylor expansion at \( \theta_0 \) with non-singular symmetric second derivative \( V_{\theta_0} \). In fact, we have \( E E_G L(\theta, gX) = E L(\theta, X) \).

Moreover, if \( \hat{\theta}_{n,G} \) is an approximate minimizer:

\[
\frac{1}{n} \sum_{i=1}^{n} E_G L(\hat{\theta}_{n,G}, gX_i) \leq \inf_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} E_G L(\theta, gX_i) + o_p(n^{-1}),
\]

and \( \hat{\theta}_{n,G} \overset{p}{\to} \theta_0 \), then \( \hat{\theta}_{n,G} \) has the following Bahadur representation

\[
\sqrt{n}(\hat{\theta}_{n,G} - \theta_0) = \frac{1}{\sqrt{n}} V_{\theta_0}^{-1} \sum_{i=1}^{n} \nabla E_G L(\theta_0, gX_i) + o_p(1).
\]

Therefore, the augmented ERM has an asymptotic variance that is reduced compared to the original ERM:

\[
\sqrt{n}(\hat{\theta}_{n,G} - \theta_0) \Rightarrow N \left( 0, V_{\theta_0}^{-1} \left[ E [\nabla L(\theta_0, \cdot) \nabla L(\theta_0, \cdot)^\top] - E \text{Cov}_G \nabla L(\theta_0, gX) \right] V_{\theta_0}^{-1} \right),
\]

and as a consequence, the relative efficiency of \( \hat{\theta}_{n,G} \) compared to \( \hat{\theta}_n \) is

\[
RE = \frac{\text{tr} \left( V_{\theta_0}^{-1} E [\nabla L(\theta_0, \cdot) \nabla L(\theta_0, \cdot)^\top] V_{\theta_0}^{-1} \right)}{\text{tr} \left( V_{\theta_0}^{-1} \left[ E [\nabla L(\theta_0, \cdot) \nabla L(\theta_0, \cdot)^\top] - E \text{Cov}_G \nabla L(\theta_0, gX) \right] V_{\theta_0}^{-1} \right)} \geq 1.
\]

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Proof. It suffices to check (a, b, c). Then the asymptotic normality follows from Theorem 4.9 and the relative efficiency formula follows from the invariance lemma.

We first check (b). We have

\[ E[(E_G \hat{L}(gX))^2] \leq E[E_G[(\hat{L}(gX))^2]] \]
\[ = E_G[E[(\hat{L}(gX))^2]] \]
\[ = E_G E\hat{L}^2 \]
\[ = E\hat{L}^2 \]
\[ < \infty, \]

where the first line is by Jensen’s inequality, the second line is by Fubini’s theorem, and the second line is by \( X = d gX \). By the assumption, we have

\[ |L(\theta_1,gx) - L(\theta_2,gx)| \leq \hat{L}(gx)\|\theta_1 - \theta_2\|. \]

Taking expectation w.r.t. \( E_G \), we have

\[ |E_G L(\theta_1,gx) - E_G L(\theta_2,gx)| \leq E_G|L(\theta_1,gx) - L(\theta_2,gx)| \leq E_G \hat{L}(gx)\|\theta_1 - \theta_2\|. \]

We then check (a). By assumption, we know that w.p. tending to one,

\[ \lim_{\delta \to 0} \frac{\left| L(\theta_0 + \delta,gX) - L(\theta_0,gX) - \delta^\top \nabla L(\theta_0,gX) \right|}{\|\delta\|} = 0. \]

Note that

\[ \frac{E_G L(\theta_0 + \delta,gX) - E_G L(\theta_0,gX) - \delta^\top E_G \nabla L(\theta_0,gX)}{\|\delta\|} \leq \frac{E_G \left| L(\theta_0 + \delta,gX) - L(\theta_0,gX) - \delta^\top \nabla L(\theta_0,gX) \right|}{\|\delta\|}, \]

and

\[ \frac{L(\theta_0 + \delta,gX) - L(\theta_0,gX) - \delta^\top \nabla L(\theta_0,gX)}{\|\delta\|} \leq \hat{L}(gX) + \|\nabla L(\theta_0,gX)\|. \]

When checking (b), we have proved that \( (x,g) \mapsto \hat{L}(gx) \) is in \( L^2(\mathbb{P} \times \mathbb{Q}) \), and hence \( g \mapsto \hat{L}(gx) \) is in \( L^1(\mathbb{Q}) \) for \( \mathbb{P} \)-a.e. \( x \). On the other hand, in view of the existence of \( E \nabla L(\theta_0,\cdot) \nabla L(\theta_0,\cdot)^\top \), we have \( E\|\nabla L(\theta_0,\cdot)\|^2 < \infty \). A similar argument shows that \( (x,g) \mapsto \|\nabla L(\theta_0,gx)\| \) is in \( L^2(\mathbb{P} \times \mathbb{Q}) \) and thus \( g \mapsto \|\nabla L(\theta_0,gx)\| \) is in \( L^1(\mathbb{Q}) \) for \( \mathbb{P} \)-a.e. \( x \). In short, the RHS in the above display is dominated by a \( L^1(\mathbb{Q}) \) function and by dominated convergence we have

\[ \liminf_{\delta \to 0} \frac{E_G \left| L(\theta_0 + \delta,gX) - L(\theta_0,gX) - \delta^\top \nabla L(\theta_0,gX) \right|}{\|\delta\|} = \frac{E_G \liminf_{\delta \to 0} \left| L(\theta_0 + \delta,gX) - L(\theta_0,gX) - \delta^\top \nabla L(\theta_0,gX) \right|}{\|\delta\|} = 0, \]

which is sufficient to conclude (a).

We finally check (c). Since \( gX = d X \), for any \( \theta \in \Theta \) we have \( E_L(\theta,gX) = E_L(\theta,X) \). Expanding \( E_L(\theta,x) \) around \( \theta_0 \) gives,

\[ E_L(\theta,gx) = E_L(\theta,gx) + \frac{1}{2}(\theta - \theta_0)^\top V_{\theta_0}(\theta - \theta_0) + o(\|\theta - \theta_0\|^2), \]

where the second and higher order term does not depend on \( G \). So taking expectation w.r.t. \( E_G \) and invoking Fubini concludes (c).

\[ \square \]
Figure 4: Computing the average covariance $\mathbb{E} \text{Cov}_G \nabla L(gX)$ of the gradient of the loss over an orbit.

**Interpretation.** The reduction in covariance is governed by $\mathbb{E} \text{Cov}_G \nabla L(\theta_0, gX)$. This is the average covariance of the gradient $\nabla L$ along the orbits $G \cdot x$. If the gradient varies a lot along the orbits, then augmentation gains a lot of efficiency. This makes sense, because this procedure effectively denoises the gradient, making it more stable. See Figure 4 for an illustration.

Alternatively, the inner term in the covariance of aMLE can also be written as $\text{Cov} \mathbb{E}_G \nabla L(\theta_0, gX)$. This is the covariance matrix of the orbit-average gradient, and similarly to above, augmentation effectively denoises and reduces it. Based on our earlier results, we can also write it as

$$\text{Cov} \mathbb{E}_G \nabla L(\theta_0, gX) = \mathbb{E}_G \mathbb{E} \nabla L(\theta_0, X) \nabla L(\theta_0, gX)^\top.$$  

This interpretation shows that it can be viewed as the average correlation (covariance) of the gradients $\nabla L(\theta_0, X)$ and $\nabla L(\theta_0, gX)^\top$.

**Understanding the Bahadur representation.** It is worth to understand the form of the Bahadur representations. For the ERM, we sum the terms $f(X_i) \equiv \nabla L(\theta, X_i)$, while for the augmented ERM, we sum the terms $\bar{f}(X_i) = \mathbb{E}_G L(\theta_0, gX_i)$. Thus, even in the Bahadur representation we can see clearly that the effect of data augmentation is to average the gradients over the orbits.

**Statistical inference.** It follows automatically from our theory that statistical inference for $\theta$ can be performed in the usual way. Specifically, assuming that $\theta \to L(\theta, x)$ is twice differentiable at $\theta_0$ on a set of full measure, we will have that $V_{\theta_0} = \mathbb{E} \nabla^2 L_{\theta_0} (X)$. We can then we can compute the plug-in estimator of $V_{\theta_0}$:

$$\hat{V}_{\theta_0} = \frac{1}{n} \sum_{i=1}^n \nabla^2 L(\hat{\theta}_{n,G}, X_i).$$

Let us also define the plug-in estimator of the averaged Fisher information:

$$\hat{T}_{\theta_0} = \frac{1}{n} \sum_{i=1}^n \nabla L(\hat{\theta}_{n,G}, X_i) \nabla L(\hat{\theta}_{n,G}, X_i)^\top.$$  

We can then define the plug-in covariance estimator

$$\hat{\Sigma} = \hat{V}_{\theta_0}^{-1} \hat{T}_{\theta_0} \hat{V}_{\theta_0}^{-1}.$$  

This leads to the following:
Corollary 4.5 (Statistical inference with the augmented estimator). Assume the same conditions as in Lemma 4.10 and Theorem 4.9. Assume in addition that \( \theta \rightarrow L(\theta, x) \) is twice differentiable at \( \theta_0 \) on a set of full \( x \)-measure, and that each entry of the Hessian \( \nabla^2 L(\theta_0, \cdot) \) is in \( L^1(\mathbb{P}) \). Assume that for both of the functions \( F_i, i = 1, 2 \) \( F_1(\theta, x) = \nabla^2 L(\theta, x) \) and \( F_2(\theta, x) = \nabla L(\theta, x)\nabla L(\theta, x)^T \) there exist \( L^1(\mathbb{P}) \) functions \( L_i \) such that for every \( \theta_1, \theta_2 \) in a neighborhood of \( \theta_0 \), we have

\[
\|F_i(\theta_1, x) - F_i(\theta_2, x)\| \leq L_i(x)\|\theta_1 - \theta_2\|.
\]

Then we have:
\[
\hat{V}_{\theta_0} \rightarrow_p V_{\theta_0}, \text{ and } \hat{I}_{\theta_0} \rightarrow_p I_{\theta_0}.
\]
Therefore, we have the asymptotic normality

\[
\sqrt{n} \Sigma^{-1/2}(\hat{\theta}_{a,G} - \theta_0) \Rightarrow \mathcal{N}\left(0, I\right).
\]

Hence, statistical inference for \( \theta_0 \) can be performed in the usual way, constructing normal confidence intervals and tests based on the asymptotic pivot.

The proof is quite direct and we omit it for brevity.

4.2.4 Implications for low-dimensional MLE

Now we consider the special case of maximum likelihood estimation in a model \( \{\mathbb{P}_\theta : \theta \in \Theta\} \). Let \( p_\theta \) be corresponding densities with respect to a common dominating measure. Assume our data \( X_1, \ldots, X_n \) are i.i.d. from \( \mathbb{P}_{\theta_0} \). Let \( \ell_\theta = \log p_\theta \), which will be our criterion function:

\[
\hat{\theta}_{\text{MLE}} \in \arg \max_{\theta \in \Theta} \sum_{i=1}^n \ell_\theta(X_i).
\]

Classical theory regarding MLE starts by assuming the model is differentiable in quadratic mean (q.m.d.), under which the score function \( \nabla \ell_\theta \) exists with \( \mathbb{E}_{\theta_0} \nabla \ell_{\theta_0} = 0 \), and the Fisher information at \( \theta_0 \), \( I_{\theta_0} = \mathbb{E}_{\theta_0} \nabla \ell_{\theta_0} \nabla \ell_{\theta_0}^T \), exists.

We now assume \( gX =_d X \) for \( X \sim \mathbb{P}_{\theta_0} \), or equivalently \( p_{\theta_0}(g^{-1}x) / \det g = p_{\theta_0}(x) \). We can define the augmented MLE estimator as

\[
\hat{\theta}_{a,\text{MLE}} \in \arg \max_{\theta \in \Theta} \sum_{i=1}^n \mathbb{E}_G \ell_\theta(gX_i).
\]

If the group acts orthogonally, we have \( p_{\theta_0}(gx) = p_{\theta_0}(x) \) and \( \ell_{\theta_0}(gx) = \ell_{\theta_0}(x) \). It is important to note that in general,

\[
\nabla \ell_{\theta_0}(gx) \neq \nabla \ell_{\theta_0}(x).
\]

To be clear, this is because we cannot differentiate the identity \( \ell_{\theta_0}(gx) = \ell_{\theta_0}(x) \) with respect to \( \theta_0 \), as it does not necessarily hold in an open neighborhood of \( \theta_0 \). If it holds in an open neighborhood, then we can differentiate and we get the identity for the score. However, it may only hold in a lower dimensional submanifold locally around \( \theta_0 \), in which case we can effectively reduce the dimensionality of the problem by constrained/augmented MLE, thus gaining efficiency. This is described below.

Corollary 4.6 (Augmentation improves MLE). Assume \( \Theta \) is open. Assume the map \( (g, X) \mapsto \ell_\theta(gX) \) is in \( L^1(\mathbb{P}_{\theta_0} \times \mathbb{Q}) \). Suppose the model \( \{\mathbb{P}_\theta : \theta \in \Theta\} \) is q.m.d. at \( \theta_0 \). Furthermore, suppose that there exists a \( L^2(\mathbb{P}_{\theta_0}) \) function \( \bar{\ell} \) such that for every \( \theta_1, \theta_2 \) in a neighborhood of \( \theta_0 \), we have

\[
|\ell_{\theta_1}(x) - \ell_{\theta_2}(x)| \leq \bar{\ell}(x)\|\theta_1 - \theta_2\|.
\]

If the Fisher information \( I_{\theta_0} = \mathbb{E}_{\theta_0} \nabla \ell_{\theta_0} \nabla \ell_{\theta_0}^T \) is non-singular and \( \hat{\theta}_{\text{MLE}}, \hat{\theta}_{a,\text{MLE}} \) are both consistent, then

\[
\sqrt{n}(\hat{\theta}_{\text{MLE}} - \theta_0) \Rightarrow \mathcal{N}(0, I_{\theta_0}^{-1})
\]

\[
\sqrt{n}(\hat{\theta}_{a,\text{MLE}} - \theta_0) \Rightarrow \mathcal{N}\left(0, I_{\theta_0}^{-1}\left(I_{\theta_0} - \mathbb{E}_{\theta_0} \text{Cov}_G \nabla \ell_{\theta_0}(gX)\right)I_{\theta_0}^{-1}\right).
\]
Figure 5: Projection into local tangent space

and the relative efficiency of $\hat{\theta}_{a\text{MLE}}$ compared to $\hat{\theta}_{\text{MLE}}$ is

$$RE = \frac{\text{tr}(I_{\theta_0}^{-1})}{\text{tr}(I_{\theta_0}^{-1}) - \text{tr}
\left(I_{\theta_0}^{-1}\left(\mathbb{E}_{\theta_0}\text{Cov}_G\nabla\ell_{\theta_0}(gX)\right)I_{\theta_0}^{-1}\right)} \geq 1.$$  

Moreover, the aMLE has the following Bahadur representation

$$\sqrt{n}(\hat{\theta}_{a\text{MLE}} - \theta_0) = \frac{1}{\sqrt{n}}I_{\theta_0}^{-1}\sum_{i=1}^{n}\nabla\mathbb{E}_G\ell_{\theta_0}(gX_i) + o_{P_{\theta_0}}(1).$$

Proof. Inspecting the proof of Theorem 5.39 in Van der Vaart (1998) gives that the conditions in Proposition 4.4 are satisfied with $L_{\theta} = -\ell_{\theta}$. So the desired result follows directly.

We also mention that data augmentation can also be analyzed in some high-dimensional M-estimation problems. If variable selection consistency holds, then the problems can be reduced to low-dimensional ones, and the same asymptotic variance formulas hold, see e.g., Wainwright (2019). Then augmentation will lead to benefits as above.

### 4.2.5 Invariance on a submanifold

Consider the invariant subspace of the parameter space $\Theta$, defined as

$$\Theta_G = \{\theta \in \Theta : gX = X \forall g \in G, \text{where } X \sim P_{\theta}\}.$$  

If this subset is small, we expect augmentation to be very efficient. Continuing to assume that the whole parameter set $\Theta$ is an open subset of $\mathbb{R}^p$, we identify $\Theta_G \subseteq \Theta$ with a smooth submanifold of $\mathbb{R}^p$. From Corollary 4.6, we see that the efficiency gain is characterized by

$$\mathbb{E}_{\theta_0}\text{Cov}_G(\nabla\ell_{\theta_0}(gX)).$$

We will investigate the magnitude of this quantity. For every $\theta \in \Theta_G$, we have $p_{\theta}(g^{-1}x)/\det g = p_{\theta}(x)$, so that

$$\ell_{\theta}(gx) + \log \det g = \ell_{\theta}(x), \forall g \in G.$$  

The following lemma says that we can decompose $\nabla\ell_{\theta_0}(gx)$ into a tangential part and orthogonal part. See Figure 5 for an illustration.

**Lemma 4.11.** Let $P_G$ be the orthogonal projection operator onto the tangent space of the manifold $\Theta_G$ at the point $\theta_0$, and let $P_G^\perp = \text{Id} - P_G$. Then we can decompose

$$\nabla\ell_{\theta_0}(gx) = P_G\nabla\ell_{\theta_0}(gx) + P_G^\perp\nabla\ell_{\theta_0}(gx),$$
and the tangential part is invariant:

\[ \nabla_x g(x) = \nabla_x h(x) \quad \forall g \in G. \]

**Proof.** Let \( T_p M \) be the tangent space of \( M \) at the point \( p \). The inclusion map from \( \Theta_G \) to \( \mathbb{R}^p \) is an immersion. So we can decompose \( T_{\theta_0} \mathbb{R}^p = T_{\theta_0} \Theta_G \oplus (T_{\theta_0} \Theta_G)_{\perp} \), i.e., the direct sum of the tangent space of \( \Theta_G \) at \( \theta_0 \) and its orthogonal complement. Hence the decomposition is valid. Now as \( \ell(\theta_0(x)) + \log \det g = \ell(x) \) for any \( \theta \in \Theta_G \), it is clear that the gradient of \( \ell_{\theta_0} \) w.r.t. \( \Theta_G \) is invariant. \( \Box \)

Then simple calculations give the following result:

**Proposition 4.7.** Under the notations of Lemma 4.11 and assumptions of Proposition 4.4, we have

\[ \mathbb{E}_{\theta_0} \text{Cov}(\nabla_x \ell_{\theta_0}(gX)) = \mathbb{E}_{\theta_0} \text{Cov}(P_G \nabla_x \ell_{\theta_0}(gX)). \]

**Proof.** Using that \( P_G \nabla_x \ell_{\theta_0}(gX) = P_G \nabla_x \ell_{\theta_0}(X) \), we have

\[
\mathbb{E}_{\theta_0} \text{Cov}(\nabla_x \ell_{\theta_0}(gX)) = \mathbb{E}_{\theta_0} \text{Cov}(P_G \nabla_x \ell_{\theta_0}(gX)) = \mathbb{E}_{\theta_0} \text{Cov}(P_G \nabla_x \ell_{\theta_0}(X)) = \mathbb{E}_{\theta_0} \text{Cov}(P_G \nabla_x \ell_{\theta_0}(gX)).
\]

A few observations are in order:

1. If \( \Theta_G \) contains an open neighborhood of \( \theta_0 \), then \( P_G = \text{Id} \), so that \( \mathbb{E}_{\theta_0} \text{Cov}(\nabla_x \ell_{\theta_0}(gX)) = 0 \). This means augmentation does not gain us anything;

2. The larger the tangential part is, the smaller the orthogonal part will be, and the less we will gain from augmentation.

**Tangential part and invariance.** Does the tangential part capture everything that is invariant? Specifically, above we have seen two different operators that capture part of the invariant component of the score, the conditional expectation over orbits \( \mathbb{E}_G \) and the projection into the tangent space \( P_G \). Is it true that \( \mathbb{E}_G = P_G \)? We will see that this is not true in general.

Let us consider a special case, where \( \theta = (\theta_1, \theta_2) \), and the constrained set \( \Theta_G \) is characterized by \( \theta_2 = 0 \). We recall the known behavior of cMLE in this case (see e.g., Van der Vaart, 1998). Let us write the score function as \( \nabla_\theta \ell_\theta(x) = (\nabla_{\theta_1} \ell_{\theta_1}(x), \nabla_{\theta_2} \ell_{\theta_2}(x)) \).

The MLE has asymptotic covariance matrix \( I_\theta^{-1} \), where

\[
I_\theta = \mathbb{E}_\theta \nabla_\theta \ell_\theta \nabla_\theta^\top \ell_\theta = \mathbb{E}_\theta \begin{bmatrix} \nabla_{\theta_1} \ell \cdot \nabla_{\theta_1} \ell^\top, \nabla_{\theta_1} \ell \cdot \nabla_{\theta_2} \ell^\top \\ \nabla_{\theta_1} \ell \cdot \nabla_{\theta_2} \ell^\top, \nabla_{\theta_2} \ell \cdot \nabla_{\theta_2} \ell^\top \end{bmatrix} = \begin{bmatrix} I_{11}(\theta), I_{12}(\theta) \\ I_{21}(\theta), I_{22}(\theta) \end{bmatrix}.
\]

The MLE constrained to \( \theta_2 = 0 \) has asymptotic covariance matrix \( J_{\theta_1}^{-1} \), where

\[
J_{\theta_1} = \mathbb{E}_{(\theta_1,0)} \nabla_{\theta_1} \ell_{(\theta_1,0)} \nabla_{\theta_1}^\top \ell_{(\theta_1,0)} = I_{11}(\theta_1,0).
\]

It is well known that the cMLE is more efficient than the MLE. This is because \( J_{\theta_1}^{-1} \leq [I_\theta^{-1}]_{11} \). Using the Schur complement formula, and omitting the \( \theta \) symbols, this is in turn equivalent to \( I_{11}^{-1} \leq [I_{11} - I_{12}I_{22}^{-1}I_{21}]^{-1} \), which is true. The tangent space is exactly \( \Theta_1 = \{(x,0) : x \in \mathbb{R}^q\} \), so

\[
P_G \nabla_\theta \ell_\theta(X) = \begin{bmatrix} \nabla_{\theta_1} \ell_{\theta_1}(X) \\ 0 \end{bmatrix}.
\]

Now, since \( \mathbb{E}_G \) is a conditional expectation, we have that \( \mathbb{E}_G \nabla_\theta \ell_\theta \) and \( \nabla_\theta \ell_\theta - \mathbb{E}_G \nabla_\theta \ell_\theta \) are uncorrelated. Hence, if \( \mathbb{E}_G \) equals \( P_G \), then \( \nabla_\theta \ell_\theta \) and \( \nabla_\theta \ell_\theta \) are uncorrelated, so that \( I_{12}(\theta) = 0 \). Conversely, if those two quantities are uncorrelated, then \( P_G \nabla_\theta \ell_\theta \) must capture everything that is invariant. So we obtained the following proposition.
**Proposition 4.8.** (Connection between expectation $E_G$ and tangent space projection $P_G$) Suppose that the parameter has two blocks, $\theta = (\theta_1, \theta_2)$, and the constrained set $\Theta_G$ is characterized by $\theta_2 = 0$. Then the conditional expectation $E_G$ over orbits equals the projection $P_G$ into the tangent space at some $\theta$ if and only if the two parameter blocks are orthogonal, i.e., $I_{12}(\theta) = 0$.

**aMLE vs cMLE.** How does the augmented MLE compare to the constrained MLE? If the true parameter belongs to the interior of the parameter set, $\theta_0 \in \text{int}\Theta_G$, then the asymptotic behavior of the two is the same. So augmentation is more computationally efficient than $\hat{\theta}_{cMLE}$, while having the same statistical efficiency. If $\Theta_G$ is a singleton, the constrained MLE gives the exact answer $\theta_0$. In comparison the augmented MLE gains some efficiency but in general will not recover $\theta_0$ exactly.

What happens to constrained MLE when the dimension of $\Theta$ is somewhere between 0 and $p$? The behavior of the constrained MLE should be characterized by the Fisher information restricted to the invariant submanifold. In general, it seems that the two are not easy to compare. We can get the following result.

**Proposition 4.9** (Relation between $aMLE$ and $cMLE$ in parametric models that decompose) Suppose that the parameter has two blocks, $\theta = (\theta_1, \theta_2)$, and the constrained set $\Theta_G$ is characterized by $\theta_2 = 0$. Denote by $I_G := \text{Cov} \mathbb{E}_G \nabla_0 (gX)$ the covariance of the average gradient. Then the aMLE is asymptotically more efficient than the cMLE if and only if the following matrix is PSD:

$$M_\theta = \begin{bmatrix} I_{11}^{-1} & (I^{-1})_{11} \\ (I^{-1})_{11} & I_G^{-1} \end{bmatrix}.$$ 

For clarity, here the notation $(I^{-1})_{11}$ refers to the submatrix of $I^{-1}$ corresponding to the rows indexed by the coordinates of $\theta_1$.

**Proof.** From our theory we know that the asymptotic covariance matrix of cMLE for estimating parameters $\theta = (\theta_1, \theta_2)$ is $I^{-1} I_G^{-1}$, while that of aMLE for estimating $\theta_1$ is $I_{11}^{-1}$. Thus aMLE is asymptotically more efficient than the cMLE if and only if

$$I_{11}^{-1} \geq [I^{-1} I_G^{-1}]_{11}.$$ 

Denoting $K := (I^{-1})_{11}$, this is equivalent to

$$I_{11}^{-1} \geq K I_G K^\top.$$ 

Using the Schur complement formula, this is equivalent to the statement that the Shur complement of the matrix $I_G^{-1}$ in the matrix $M_\theta$ is PSD, where $M_\theta$ equals

$$M_\theta = \begin{bmatrix} I_{11}^{-1} & K \\ K^\top & I_G^{-1} \end{bmatrix}.$$ 

Now, the top left block of this matrix, $I_{11}^{-1}$, is PSD. Thus, from the properties of Schur complements, the entire matrix $M_\theta$ is also PSD. Therefore, the condition is equivalent to the matrix $M_\theta$ being PSD.

4.3 Finite augmentations

The above arguments refer to the augmented estimator that involves integrals over $G$, which are intractable if $G$ is infinite. Therefore, it is of interest to understand what happens for a finite approximation. It turns out that we can repeat the above arguments with minimal changes. Specifically, given a function $f(x)$, we can define $f_k(x) = k^{-1} \sum_{j=1}^{k} f(g_j x)$, where $g_j$ are arbitrary elements of $G$. Similarly to before, we find that the mean is preserved, while the variance is reduced, in the following way:

1. $\mathbb{E}_\mathcal{P} f(X) = \mathbb{E}_\mathcal{P} f_n(X)$.

2. $\text{Cov}_\mathcal{P} f(X) = \text{Cov}_\mathcal{P} f_n(X) + \mathbb{E}_\mathcal{P} \text{Var}_k[f(g_1 X), \ldots, f(g_k X)]$, where $\text{Var}_k(a_1, \ldots, a_k)$ is the variance of the $k$ numbers $a_i$. 

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Repeating the above arguments, this shows that the finitely augmented estimators have reduced mean squared errors. This holds regardless of the augmentations \( g_i \) chosen, even if they are deterministic. Moreover, the efficiency gain is governed by the average variance of

1. the numbers \( \hat{\theta}(g_i X) \), for plug-in augmentation.
2. the numbers \( \nabla L(\theta, g_i X) \), for augmented ERM.

This suggests that we may be able to get better augmentations if we choose \( g_i \) to “vary a lot” in the appropriate variance metric.

5 Examples

In this section we give several examples of models where symmetry occurs, and we characterize data augmentation and various other estimators.

5.1 Exponential families

We start with exponential families, which are a fundamental class of models in statistics (e.g., Lehmann and Casella, 1998; Lehmann and Romano, 2005). Suppose \( X \sim \mathbb{P}_\theta \) is distributed according to an exponential family, such that

\[
\ell_\theta(X) = \theta^\top T(X) - A(\theta),
\]

where \( T(X) \) is the sufficient statistic, \( \theta \) is the natural parameter, \( A(\theta) \) is the log-partition function. The density is with respect to some \( \sigma \)-finite measure on \( \mathbb{R}^p \). Then we have the score function \( \nabla \ell_\theta(X) = T(X) - \nabla A(\theta) \), and the Fisher information

\[
I_\theta = \text{Cov}[T] = \nabla^2 A(\theta).
\]

Given invariance with respect to a group \( G \), the asymptotic covariance matrix of the aMLE equals

\[
I_\theta^{-1} \theta^\top J_\theta I_\theta^{-1} \theta,
\]

where \( J_\theta \) is the covariance of the orbit-averaged sufficient statistic

\[
J_\theta = \text{Cov}_G[T(gX)].
\]

Assuming a linear action by the group \( G \), and working in a matrix representation of \( G \), the invariant parameter set \( \Theta_G \) consists of those parameters \( \theta \) for which

\[
\theta^\top [T(gX) - T(x)] + v(g) = 0, \quad \forall g, x.
\]

Here \( v(g) = \log \det g \) is the log-determinant. This is a set of linear equations. Moreover, the log-likelihood is concave, and hence the constrained MLE estimator can in principle be computed as the solution to the following convex optimization problem.

\[
\hat{\theta}_{cMLE} \in \arg \max_{\theta} \theta^\top T(X) - A(\theta)
\]

s.t. \( \theta^\top [T(gX) - T(x)] + v(g) = 0, \quad \forall g, x. \)

Assume that \( \Theta = \mathbb{R}^p \), so that the exponential family is well defined for all natural parameters, and that \( \nabla A \) is invertible on the range of \( \mathbb{E}_G T(gX) \). The KKT (or Lagrange) conditions reduce to

\[
\hat{\theta}_{cMLE} \in [\nabla A]^{-1}(T(X) + \text{span}(T(gz) - T(z) : z \in \mathbb{R}^k, g \in G))
\]

s.t. \( \theta^\top [T(gx) - T(x)] + v(g) = 0, \quad \forall g, x. \)

Meanwhile, augmented MLE is the solution of the optimization problem where we replace the sufficient statistic \( T(x) \) by \( T(x) = \mathbb{E}_G T(gX) \).

\[
\hat{\theta}_{aMLE} \in \arg \max_{\theta} \theta^\top \mathbb{E}_G T(gX) - A(\theta)
\]

We then have \( \hat{\theta}_{aMLE} = [\nabla A]^{-1}(\mathbb{E}_G T(gX)) \). Therefore, for exponential families we were able to give more concrete expressions for the augmented and constrained MLEs.

**Gaussian mean.** Consider now the important special case of Gaussian mean estimation. Suppose that \( X \) is a standard Gaussian random variable, so that \( A(\theta) = ||\theta||^2/2 \), and \( T(x) = x \). Then, consider those
parameter values left invariant by the linear action of the group, and define the invariant subspace of the parameter space under the action of $G$, $I(G) = \{v : g^\top v = v, \forall g \in G\}$. Recalling that the group acts in a linear way, we have

\[
\hat{\theta}_{cMLE}(X) = P_{I(G)}(X),
\]
\[
\hat{\theta}_{aMLE}(X) = E_G[g] \cdot X.
\]

In fact, the following argument shows that the two estimators coincide when our group $G$ is represented by orthogonal matrices. Let $C = E_G[g]$. By orthogonality, for each $g$ we have that $g^\top g^{-1}$ is also in $G$. Hence, the matrix $C$ is symmetric. Then for any $v \in I(G)$, we have $Cv = E_G[gv] = E_G[v] = v$. Thus, $C$ has $I(G)$ as an invariant subspace. Moreover, for any $w \in I(G)^\perp$, we have $Cw = E_G[gw] = E_G[0] = 0$. Hence, $C$ is exactly the orthogonal projection into the subspace $I(G)$. Therefore, we have shown:

**Proposition 5.1.** If $X$ is standard Gaussian, and $G$ is a subgroup of the orthogonal group, then both $aMLE$ and $cMLE$ are equal to the projection into the invariant subspace of $G$. In particular, their risk equals $\dim I(G)$.

For instance, suppose $G = \{I, -I\}$ is the reflection group. Then it is clear that $I(G) = \{0\}$, and so both the cMLE and aMLE are identically equal to zero.

On the other hand, the marginal MLE (mMLE) is a different object, even in the one-dimensional case. Suppose that $X \sim \mathcal{N}(\theta, 1)$, and we consider the reflection group $G = \{1, -1\}$. The marginal distribution of the data is a Gaussian mixture model

\[ Z \sim \frac{1}{2} [\mathcal{N}(\theta, 1) + \mathcal{N}(\theta, 1)]. \]

So the mMLE fits a mixture model, solving

\[
\hat{\theta}_{\text{mMLE}, n} = \arg\max_{\theta} \sum_{i=1}^{n} \log \left( \int_G p_\theta(gX_i) dQ(g) \right) \\
= \arg\min_{\theta} \sum_{i=1}^{n} \log \left( \frac{1}{2} [p_\theta(X_i) + p_\theta(-X_i)] \right) \\
= \arg\min_{\theta} \sum_{i=1}^{n} \log \left( \exp[-(X_i - \theta)^2/2] + \exp[-(-X_i - \theta)^2/2] \right)
\]

The solution to this is not necessarily identically equal to zero, and in particular it does not agree with the cMLE and aMLE.

**Numerical results.** We present some numerical results to support our theory. We consider $X \sim \mathcal{N}(\mu, I_d)$, and invariance to the reflection group. This is a simple model of invariance, which occurs for instance in objects like faces.

In Figure 6, we show the results of two experiments. On the left figure, we show the histograms of the mean squared errors (normalized by dimension) of the MLE and the augmented MLE on a $d = 100$ dimensional Gaussian problem. We repeat the experiment $n_{MC} = 100$ times. We see that the MLE has average MSE roughly equal to unity, while the augmented MLE has average MSE roughly equal to one half. Thus, data augmentation reduces the MSE two-fold. This confirms our theory.

On the right figure, we change the model to each coordinate $X_i$ of $X$ being sampled independently as $X_i \sim \text{Poisson}(\lambda)$. We show that the relative efficiency (the relative decrease in MSE) of the MLE and the augmented MLE is roughly equal to two regardless of $\lambda$. This again confirms our theory.

### 5.2 Nonlinear regression and two-layer neural networks

We consider a nonlinear regression problem where we observe a random sample $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \subseteq \mathbb{R}^d \times \mathbb{R}$ from the law of a random vector $(X, Y)$. This follows the model:

\[ Y = f(\theta_0, X) + \varepsilon, \quad \varepsilon \perp X, \quad \mathbb{E}\varepsilon = 0, \]
Figure 6: Plots of the increase in efficiency achieved by data augmentation in a *flip symmetry* model.

where $\theta_0 \in \mathbb{R}^p$. We have a group $G$ acting on $\mathbb{R}^d \times \mathbb{R}$ only through $X$:

$$g(X, Y) = (gX, Y),$$

and the invariance is characterized by

$$(gX, Y) =_d (X, Y).$$

In regression or classification problems in deep learning, we typically apply the augmentations conditionally on the outcome or class label. This corresponds to the conditional invariance

$$(gX|Y = y) =_d (X|Y = y).$$

Since this holds conditionally for each $y$, we deduce that it also holds jointly, i.e., $(gX, Y) =_d (X, Y)$, and unconditionally, i.e., $gX =_d X$. Thus, each type of invariance (conditional, joint, and unconditional) hold. What does the invariance say? Consider events of the form $A \times B$. By invariance we have

$$P(X \in A, Y \in B) = P(gX \in A, Y \in B).$$

If we take $Y = \mathbb{R}$, we deduce that $X$ is invariant in distribution. Then, considering $A$ such that $P(X \in A) > 0$, we find that the conditional distribution of $Y = y|X \in A$ is invariant. In other words, the meaning of the invariance relation is two-fold:

1. the feature vector $X$ is invariant: $X =_d gX$ for any $g \in G$;

2. the noiseless label is invariant: $P(Y = y|x) = P(Y = y|x = gx)$ for any non-random $x \in \mathbb{R}^d$ and any $g \in G$.

This is what we would expect in the applications we have in mind. We think of $x$ as an image. The group consists of rotations, flips, etc., that act on images. Then we would expect that, not only the distribution on $X$ is invariant, but also the label is preserved provided there is no random error.

**Least squares.** For the least squares estimator, the loss function is

$$L(\theta, X, Y) = (Y - f(\theta, X))^2.$$

The population risk is

$$\mathbb{E}L_\theta(X, Y) = \mathbb{E}(Y - f(\theta_0, X) + f(\theta_0, X) - f(\theta, X))^2 = \mathbb{E}(f(\theta_0, X) - f(\theta, X))^2 + \sigma^2.$$

We will denote by $\sigma^2 := \mathbb{E}\epsilon^2$ the noise variance. Under reasonable assumptions, the minimizer $\hat{\theta}_{ERM}$ of $\theta \mapsto \sum_{i=1}^n L(\theta, X_i, Y_i)$ is consistent, see e.g., Example 5.27 of Van der Vaart (1998). Similarly, under reasonable smoothness conditions, we would have

$$\mathbb{E}L(\theta, X, Y) = \sigma^2 + \frac{1}{2} \mathbb{E} \left[ (\theta - \theta_0)^\top \left( 2\nabla f(\theta_0, X)\nabla f(\theta_0, X)^\top \right) (\theta - \theta_0) \right] + o(\|\theta - \theta_0\|^2),$$

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where $\nabla f(\theta, X)$ is the gradient w.r.t. $\theta$. This suggests that we can apply Theorem 4.9 with $V_{\theta_o} = 2E\nabla f(\theta_0, X)\nabla f(\theta_0, X)^\top$ and $V L(\theta_0, X, Y) = -2(Y - f(\theta_0, X))\nabla f(\theta_0, X) = -2\varepsilon \nabla f(\theta_0, X)$, which gives (with the Fisher information $I_\theta = E\nabla f(\theta, X)\nabla f(\theta, X)^\top$)

$$\sqrt{n}(\hat{\theta}_{\text{ERM}} - \theta_0) \Rightarrow N\left(0, V_{\theta_0}^{-1}E\left[4\varepsilon^2 \nabla f(\theta_0, X)\nabla f(\theta_0, X)^\top\right]V_{\theta_0}^{-1}\right) = d N\left(0, \sigma^2 I_{\theta_0}^{-1}\right).$$

**Augmented least squares.** On the other hand, the augmented ERM estimator is the minimizer $\hat{\theta}_{a\text{ERM}}$ of $\theta \mapsto \sum_{i=1}^n E_G L(\theta, gX_i, Y_i)$. Now applying Proposition 4.4 gives

$$\sqrt{n}(\hat{\theta}_{a\text{ERM}} - \theta_0) \Rightarrow N(0, \Sigma_{a\text{ERM}}),$$

with the asymptotic covariance being

$$\Sigma_{a\text{ERM}} = \sigma^2 I_{\theta_0}^{-1} - V_{\theta_0}^{-1}E\left[\text{Cov}_G \nabla L(\theta_0, gX, Y)\right]V_{\theta_0}^{-1}$$

$$= \sigma^2 I_{\theta_0}^{-1} - V_{\theta_0}^{-1}E\left[\text{Cov}_G(Y - f(\theta_0, gX))\nabla f(\theta_0, gX)\right]I_{\theta_0}^{-1}$$

$$= \sigma^2 \left(I_{\theta_0}^{-1} - V_{\theta_0}^{-1}E\left[\text{Cov}_G \nabla f(\theta_0, gX)\right]I_{\theta_0}^{-1}\right),$$

where we used $f(\theta_0, gX) = f(\theta_0, x)$ in the second to last line.

**Two-layer neural network.** As an example, consider a two-layer neural network

$$f(\theta, x) = \beta^\top \sigma(Wx).$$

Here $x$ is a $d$-dimensional input, $W$ is a $p \times d$ weight matrix, $\sigma$ is a nonlinearity applied elementwise to the preactivations $Wx$. Then $A := \sigma(Wx)$ are the activations of the first layer. Finally $\beta$ is a $p \times 1$ vector containing the weights of the second layer. The overall parameters are $\theta = (\beta, W)$. For simplicity, let us focus on the case where $\beta = 1_p$ is the all ones vector. This will simplify the expressions for the gradient. We can then write $f(W, x) = 1^\top \sigma(Wx)$.

**Calculations.** We then have

$$\nabla f(W, x) = \sigma'(Wx) \cdot x^\top \in \mathbb{R}^{p \times d}.$$

We can think of the Fisher information matrix $I_\theta = E\nabla f(\theta, X)\nabla f(\theta, X)^\top$ as a tensor, i.e,

$$I_W = E(\sigma'(Wx) \cdot X^\top) \otimes (\sigma'(Wx) \cdot X^\top)$$

$$= E(\sigma'(Wx) \otimes \sigma'(Wx)) \cdot (X \otimes X)^\top.$$

The $i, j, i', j'$-th entries of this tensor are

$$I_W(i, j, i', j') = E\sigma'(W_{i'}^\top X)\sigma'(W_{i'}^\top X) \cdot X_jX_{j'}.$$

In general it seems non-obvious to compute this expectation. For instance, when $\sigma(x) = \max(x, 0)$ is the rectified linear unit (ReLU) nonlinearity, we have $\sigma'(x) = I(x \geq 0)$ (in a distributional sense), and thus, the entries are

$$I_W(i, j, i', j') = E(I(W_{i'}^\top X \geq 0) \cdot W_{i'}^\top X \geq 0) \cdot X_jX_{j'}.$$

In a model where $X \sim N(0, I_d)$, this is the covariance of two coordinates of a Gaussian restricted to an intersection of two hyperplanes, and thus has an explicit expression in terms of arc-cosines, see for instance Du et al. (2018); Arora et al. (2019). We will consider this to be a fundamental notion, and work with it in what follows. Let $h_{j,j'}(a, b) := E\sigma'(a^\top X) \geq 0 \cdot \sigma'(b^\top X) \geq 0 \cdot X_jX_{j'}$, where $X \sim N(0, I_d)$. Then $I_W(i, j, i', j') = h_{ij'}(W_i, W_{i'})$.
**Quadratic activation.** For a quadratic activation function, $\sigma(x) = x^2/2$, we can get more detailed results. We then have

$$I_W = \mathbb{E}(WXX^\top) \otimes (WXX^\top) = (W \otimes W) \cdot \mathbb{E}(XX^\top \otimes XX^\top).$$

Thus the information is a matrix product of the 4th order moment tensor of $X$. Note that for a normal distribution, most of the terms vanish. The only ones surviving belong to two classes. First, $\mathbb{E}X_iX_jX_j = 1$ if there are two distinct indices among $i, i', j, j'$, and $\mathbb{E}X_iX_jX_jX_j' = 3$ if there is one index.

**Invariance.** What happens under invariance? We need to compute $\mathbb{E}[\text{Cov}_G \nabla f(\theta, gX)]$, which depends on the nature of the invariance. A natural example is invariance to circular shifts (translation-invariance). The group acts by $gx = T_gx$, where $T_\theta$ is an operator that shifts a vector circularly by $\theta$ units. We can then write the neural network $f(W, x) = \sum_{i=1}^p h(W_i; x)$ as a sum, where $h(a, x) = \sigma(a^\top x)$. Therefore, the invariant function corresponding to $f_W$ can also be written in terms of the corresponding invariant functions corresponding to the $h$s:

$$\overline{f}(W, x) = \frac{1}{d} \sum_{g=1}^d f(W, T_gx) = \sum_{i=1}^p \overline{h}(W_i; x).$$

where $\overline{h}(a; x) = \frac{1}{d} \sum_{g=1}^d h(a; T_gx)$. We can use this representation to calculate the gradient. We first notice $\nabla h(a; x) = \sigma'(a^\top x)x$. Thus,

$$\nabla \overline{h}(a; x) = \frac{1}{d} \sum_{g=1}^d \nabla h(a; T_gx) = \frac{1}{d} \sum_{g=1}^d \sigma'(a^\top T_gx)T_gx$$

$$= \frac{1}{d} C_x \cdot \sigma'(C_x^\top a).$$

Here $C_x$ is the circulant matrix

$$C_x = [x, T_1x, \ldots, T_{d-1}x] = \begin{bmatrix} x_1, & x_d, & \ldots, & x_{d-1} \\ x_2, & x_1, & \ldots, & x_d \\ \vdots & \vdots & \ddots & \vdots \\ x_d, & x_{d-1}, & \ldots, & x_1 \end{bmatrix}.$$ 

Hence the gradient of the invariant neural network $\overline{f}(W, x)$ as a matrix-vector product

$$\nabla \overline{f}(W, x) = \begin{bmatrix} \nabla \overline{h}(W_1; x)^\top \\ \vdots \\ \nabla \overline{h}(W_p; x)^\top \end{bmatrix} = \frac{1}{d} \begin{bmatrix} \sigma'(W_1^\top C_x) \cdot C_x^\top \\ \vdots \\ \sigma'(W_p^\top C_x) \cdot C_x^\top \end{bmatrix} = \frac{1}{d} \sigma'(WC_x) \cdot C_x^\top.$$ 

So the Fisher information can also expressed in terms of matrix products

$$I_W = \mathbb{E}(\sigma'(WC) \cdot C_x^\top) \otimes (\sigma'(WC) \cdot C_x^\top)$$

$$= \mathbb{E}(\sigma'(WC) \otimes \sigma'(WC)) \cdot (C_x \otimes C_x)^\top.$$ 

For quadratic activation functions, we have

$$I_W = \frac{1}{d^2} \mathbb{E}(WC_xC_x^\top) \otimes (WC_xC_x^\top)$$

$$= (W \otimes W) \cdot \frac{1}{d^2} \mathbb{E}(C_x C_x^\top \otimes C_x C_x^\top)$$

$$= (W \otimes W) \cdot \frac{1}{d^2} \mathbb{E}(C_x \otimes C_x \cdot (C_x \otimes C_x)^\top).$$

Therefore, the efficiency gain can be characterized by the move from the 4th moment tensor of $X$ to that of $\frac{1}{\sqrt{d}} C_X$. 

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We can express our results in a simpler form using the Fourier transform. Let $F$ be the $d \times d$ Discrete Fourier Transform (DFT) matrix, with entries $F_{j,k} = d^{-1/2} \exp(-2\pi i / d \cdot (j - 1)(k - 1))$. Then $Fx$ is called the DFT of the vector $x$, and $F^{-1}y = F^\dagger y$ is called the inverse DFT. The DFT matrix is a unitary matrix with $FF^* = F^*F = I_X$. Thus $F^{-1} = F^*$. It is also a symmetric matrix with $F^\top = F$. Then the circular matrix can be diagonalized as

$$1 \sqrt{d} \begin{bmatrix} \omega & I_X \end{bmatrix} = F^* \text{diag}(Fx)F.$$

The eigenvalues of $d^{-1/2}Cx$ are the entries of $Fx$, with eigenvectors the corresponding columns of $F$.

So we can write, with $D := \text{diag}(FX)$,

$$d^{-1}C_X \otimes C_X = F^*DF \otimes F^*DF = (F \otimes F)^\top \cdot (D \otimes D) \cdot (F \otimes F) = F_2^\top D_2 F_2,$$

where $F_2 = F \otimes F$, and $D_2 = D \otimes D$ is a diagonal matrix. So

$$d^{-2}\mathbb{E}(C_X \otimes C_X) \cdot (C_X \otimes C_X)^\top = \mathbb{E}F_2^\top D_2 F_2 \cdot (F_2^\top D_2 F_2)^\top$$

$$= \mathbb{E}F_2^\top D_2 F_2 \cdot F_2^\top D_2 F_2^\top = F_2^\top \cdot \mathbb{E}D_2 F_2^\top D_2 \cdot F_2^\top.$$

Here we used that $F = F^\top$, hence $F_2^\top = (F \otimes F)^\top = F^\top \otimes F^\top = F_2$.

Now, $D_2$ can be viewed as a $d^2 \times d^2$ matrix, with diagonal entries $D_2(i,j,i,j) = D_i D_j = F_{i}^\top X \cdot F_{j}^\top X$, where $F_i$ are the rows (which are also equal to the columns) of the DFT. Thus the inner expectation can be written as an elementwise product (also known as Hadamard or odot product)

$$\mathbb{E}D_2 F_2^\top D_2 = F_2^\top \odot \mathbb{E}D_2 D_2^\top.$$

So we only need to calculate the 4th order moment tensor $M$ of the Fourier transform $FX$,

$$M_{ij\ell j'} = \mathbb{E}F_i^\top F_j^\top X \cdot F_{i'}^\top F_{j'}^\top X.$$

Let us write $r := FX$. Then by Wick’s formula,

$$\mathbb{E}f_i f_j f_{i'} f_{j'} = \mathbb{E}f_i f_j \cdot \mathbb{E}f_{i'} f_{j'} + \mathbb{E}f_i f_{i'} \cdot \mathbb{E}f_j f_{j'} + \mathbb{E}f_i f_{j'} \cdot \mathbb{E}f_j f_{i'}.$$

Now

$$\mathbb{E}f_i f_j = \mathbb{E}F_i^\top F_j X = F_i^\top \cdot \mathbb{E}XX^\top \cdot F_j = F_i^\top F_j.$$

Hence

$$M_{ij\ell j'} = F_i^\top F_j \cdot F_{i'}^\top F_{j'} + F_i^\top F_{i'} \cdot F_{j}^\top F_{j'} + F_{i'}^\top F_{i'} \cdot F_{j'}^\top F_{j'}.$$

This leads to a completely explicit expression for the average information. Recall $F_2 = F \otimes F$, and $M$ is the $d^2 \times d^2$ tensor with entries given above. Then

$$\bar{I}_W = (W \otimes W) \cdot F_2^\top \cdot (F_2^2 \odot M) \cdot F_2^\top.$$

We have obtained the following theorem:

**Theorem 5.1** (Circular shift data augmentation in two-layer networks with quadratic activation). Consider the two-layer neural network model $Y = 1^\top \sigma(WX) + \varepsilon$, where the input $X$ is a $d$-dimensional vector, $W$ is a $p \times d$ weight matrix, and $\sigma$ is a differentiable nonlinearity applied elementwise to the preactivations $WX$.

1. The Fisher information matrix $I_W = \mathbb{E} \nabla f(W, X) \nabla f(W, X)^\top$ can be viewed as a tensor

$$I_W = \mathbb{E}(\sigma'(WX) \otimes \sigma'(WX)) \cdot (X \otimes X)^\top.$$
2. If the activation function is quadratic, \( \sigma(x) = x^2/2 \), then the information is a product of the \( p^2 \times d^2 \) tensor \( W \otimes W \) and the \( d^2 \times d^4 \) 4th order moment tensor of \( X \):

\[
I_W = (W \otimes W) \cdot \mathbb{E}(XX^\top \otimes XX^\top).
\]

3. Consider now augmentations acting by circular shift. This induces translation-invariance of the network. Let \( C_v \) be the circulant matrix associated with the vector \( v \), with entries \( C_v(i, j) = v_{i+j} \). Then the augmented Fisher information, \( T_W = \mathbb{E}[\text{Cov}_G \nabla f(\theta, gX)] \), which equals the average of the orbit covariance of the gradient, has the form

\[
T_W = (W \otimes W) \cdot d^{-2}\mathbb{E}(C_X \otimes C_X) \cdot (C_X \otimes C_X)^\top.
\]

4. If the distribution of \( X \) is normal, \( X \sim \mathcal{N}(0, I_d) \), then this has the explicit form

\[
T_W = (W \otimes W) \cdot (F_2^2 \otimes M) \cdot F_2^2.
\]

Here \( F_2 = F \otimes F \) is the \( d \times d \) DFT matrix, and \( M \) is the \( d^2 \times d^2 \) tensor with entries

\[
M_{ij, ij'} = F_i^\top F_j : F_{i'}^\top F_{j'} + F_i^\top F_j' \cdot F_{i'}^\top F_j + F_i^\top F_j \cdot F_i^\top F_{j'}.
\]

This theorem shows in a precise quantitative sense how much we gain from data augmentation in a two-layer neural network. Recall that the conclusion for the low-dimensional ERM is

\[
\sqrt{n}(\widehat{W}_{ERM} - W) \Rightarrow \mathcal{N}(0, \sigma^2 I_W^{-1})
\]

\[
\sqrt{n}(\widehat{W}_{\alpha\text{ERM}} - W) \Rightarrow \mathcal{N}(0, \sigma^2 I_W^{-1}T_W I_W^{-1}).
\]

To get a sense of the magnitude of improvement, we will attempt to understand how much “smaller” \( T_W \) is compared to \( I_W \) by calculating \( \mathbb{E} \text{tr } I_W = \mathbb{E}\|WX^\top\|^2_F \). Let \( S = XX^\top \). Now \( W \sim \mathcal{N}(0, I_p \otimes S^2) \), so \( WS \sim \mathcal{N}(0, I_p \otimes S^2) \); hence, \( \mathbb{E}\|WS\|^2_F = p \text{tr } S^2 = p \text{tr } (XX^\top)^2 \). Similarly, we find \( \mathbb{E} \text{tr } T_W = p \text{tr } (C_X C_X^\top)^2/d^2 \).

**Numerical results.** In Figure 7, we show the results of an experiment where we randomly generate the input as \( X \sim \mathcal{N}(0, I_d) \). We compute the values of \( \mathbb{E} \text{tr } I_W = p \text{tr } (XX^\top)^2 \) and \( \mathbb{E} \text{tr } T_W = p \text{tr } (C_X C_X^\top)^2/d^2 \), and record their ratio. We repeat the experiment \( n_{MC} = 100 \) times. We then show the relative efficiency of aMLE with respect to MLE as a function of the input dimension \( d \). We find that the relative efficiency scales as \( RE(d) \sim d/2 \). Thus, for the efficiency gain increases as a function of the input dimension. However, the efficiency gain does not depend on the output dimension \( p \). This makes sense, as circular invariance affects and reduces only the input dimension.
Limitations. While our result does indeed concern the important case of two-layer neural networks, it does have several significant limitations. To start, we assume that the activation function is differentiable, which does not cover the important example of rectified linear unit (or ReLU) activation max(x, 0). Moreover, most of our results concern quadratic activations, which are quite limited. Also, the entire result concerns the asymptotic variance of the estimator of the weights of the neural network, which can only be sensible if the number of data points is much larger than the number of parameters. This is again a significant limitation, as many modern neural networks have larger numbers of parameters than the size of the data. Finally, this result assumes that we can optimize the weights of the neural network to consistently estimate the true weights, which is in general a hard nonconvex optimization problem to which there are only partially known solutions.

5.3 Nonlinear least squares classification

Similar calculations carry over to the classification case. We now have a random sample \{(X_1, Y_1), ..., (X_n, Y_n)\} ⊆ \mathbb{R}^d \times \{0, 1\} from the law of a random vector (X, Y), which follows the classification model:

\[
P(Y = 1 \mid X) = \sigma(f(\theta_0, X)),
\]

where \(\theta_0 \in \mathbb{R}^p, \sigma : \mathbb{R} \to [0, 1]\) is an increasing activation function, and \(f(\theta_0, \cdot)\) is a real-valued function. For example, the sigmoid \(\sigma(x) = 1/(1 + e^{-x})\) gives the logistic regression model, using features extracted by \(f(\theta_0, \cdot)\). As in the regression case, we have a group \(G\) acting on \(\mathbb{R}^d \times \{0, 1\}\) via

\[
g(X, Y) = (gX, Y),
\]

and the invariance is

\[
(gX, Y) =_d (X, Y).
\]

Invariance. The interpretation of the invariance relation is again two-fold. On the one hand, we have \(gX =_d X\). And on the other hand, for almost every (w.r.t. the law of \(X\)) \(x\), we have

\[
P(Y = 1 \mid gX = x) = P(Y = 1 \mid X = x).
\]

The LHS is \(\sigma(f(\theta_0, g^{-1}x))\), whereas the RHS is \(\sigma(f(\theta_0, x))\). This shows that for any (non-random) \(g \in G\) and \(x\), we have

\[
\sigma(f(\theta_0, gx)) = \sigma(f(\theta_0, x)).
\]

For image classification, the invariance relation says that the class probabilities stay the same if we transform the image by the group action. Moreover, since we assume \(\sigma\) is monotonically strictly increasing, applying its inverse actually gives

\[
f(\theta_0, gx) = f(\theta_0, x).
\]

Fitting the model. We consider using the least square loss to train the classifier:

\[
L(\theta, X, Y) = (Y - \sigma(f(\theta, X)))^2.
\]

Though this is not the most natural loss, in some cases it can be empirically superior to the default choices, e.g., logistic loss and hinge loss (Wu and Liu, 2007; Nguyen and Sanner, 2013). The loss function has a bias-variance decomposition:

\[
\mathbb{E}L(\theta, X, Y) = \mathbb{E}[Y - \sigma(f(\theta_0, X)) + \sigma(f(\theta_0, X)) - \sigma(f(\theta, X))]^2
\]

\[
= \mathbb{E}[Y - \sigma(f(\theta_0, X))]^2 + \mathbb{E}[\sigma(f(\theta, X)) - \sigma(f(\theta, X))]^2
\]

where the cross-term vanishes because \(\sigma(f(\theta_0, X)) = \mathbb{E}[Y | X]\). Note that

\[
\mathbb{E}[Y - \sigma(f(\theta_0, X))]^2 = \mathbb{E}[(Y - \mathbb{E}[Y | X])^2]
\]

\[
= \mathbb{E} \left[ (Y - \mathbb{E}[Y | X])^2 | X \right]
\]

\[
= \mathbb{E} \text{Var}(Y | X)
\]

\[
= \mathbb{E} \text{Bernoulli}(\sigma(f(\theta_0, X)))]
\]

\[
= \mathbb{E} \sigma(f(\theta_0, X))(1 - \sigma(f(\theta_0, X))).
\]
Meanwhile, since $\nabla \sigma(f(\theta, X)) = \sigma'(f(\theta, X))\nabla f(\theta, X)$, for sufficiently smooth $\sigma$, we have a second-order expansion of the population risk:

$$\mathbb{E}L(\theta, X, Y) = \mathbb{E}L(\theta_0, X, Y) + \frac{1}{2}(\theta - \theta_0)^T \mathbb{E}[2\sigma'(f(\theta_0, X))^2 \nabla f(\theta_0, X) \nabla f(\theta_0, X)^T](\theta - \theta_0) + o(\|\theta - \theta_0\|^2).$$

This suggests that we can apply Theorem 4.9 with $V_{\theta_0} = \mathbb{E}[2\sigma'(f(\theta_0, X))^2 \nabla f(\theta_0, X) \nabla f(\theta_0, X)^T]$ and $\nabla L(\theta, X, Y) = -2(Y - \sigma(f(\theta, X)))\sigma'(f(\theta, X))\nabla f(\theta, X)$, which gives

$$\sqrt{n}(\hat{\theta}_{ERM} - \theta_0) \Rightarrow \mathcal{N}(0, \Sigma_{ERM}),$$

where the asymptotic covariance is

$$\Sigma_{ERM} = \mathbb{E}[U_{\theta_0}(X)]^{-1}\mathbb{E}[v_{\theta_0}(X)U_{\theta_0}(X)]\mathbb{E}[U_{\theta_0}(X)]^{-1}$$

in which we defined

$$v_{\theta_0}(X) = \sigma(f(\theta_0, X)) \cdot (1 - \sigma(f(\theta_0, X)))$$

$$U_{\theta_0}(X) = \sigma'(f(\theta_0, X))^2 \nabla f(\theta_0, X) \nabla f(\theta_0, X)^T.$$

Here $v_{\theta_0}(X)$ can be viewed as the noise level, which corresponds $\mathbb{E}\varepsilon^2$ in the regression case. Also, $U_{\theta_0}(X)$ is the information, which corresponds to $\mathbb{E}\nabla f(\theta_0, X) \nabla f(\theta_0, X)^T$ in the regression case. The classification problem is a bit more involved, because the noise and the information do not decouple (they both depend on $X$). In a sense, the asymptotics of classification correspond to a regression problem with heteroskedastic noise, whose variance depends on the mean signal level.

In contrast, applying Proposition 4.4 gives

$$\sqrt{n}(\hat{\theta}_{aERM} - \theta_0) \Rightarrow \mathcal{N}(0, \Sigma_{aERM}),$$

where

$$\Sigma_{ERM} - \Sigma_{aERM} = V_{\theta_0}^{-1}\mathbb{E}\text{Cov}_G \nabla L(\theta_0, gX)V_{\theta_0}^{-1}.$$  

We now compute the gain in efficiency:

$$\mathbb{E}\text{Cov}_G \nabla L(\theta_0, gX) = \mathbb{E}\text{Cov}_G \left(2(Y - \sigma(f(\theta_0, gX)))\sigma'(f(\theta_0, gX))\nabla f(\theta_0, gX)\right)$$

$$= 4\mathbb{E}\left[(Y - \sigma(f(\theta_0, gX)))^2\text{Cov}_G \left(\sigma'(f(\theta_0, gX))\nabla f(\theta_0, gX)\right)\right]$$

$$= 4\mathbb{E}\left[v_{\theta_0}(X)\text{Cov}_G \left(\sigma'(f(\theta_0, gX))\nabla f(\theta_0, gX)\right)\right].$$

In summary, the covariance of ERM is larger than the covariance of augmented ERM by

$$\Sigma_{ERM} - \Sigma_{aERM} = \mathbb{E}[U_{\theta_0}(X)]^{-1}\mathbb{E}\left[v_{\theta_0}(X)\text{Cov}_G \left(\sigma'(f(\theta_0, gX))\nabla f(\theta_0, gX)\right)\right]\mathbb{E}[U_{\theta_0}(X)]^{-1}.$$  

**Calculations.** Most of the computations for the two-layer neural net regression carry over to classification. Recall that the two layer neural net is

$$P(Y = 1 \mid X) = f(W, X) := \sigma(\beta^T \tilde{\sigma}(WX)),$$

where $W \in \mathbb{R}^{p \times d}$ and $\tilde{\sigma}$ is a nonlinearity applied elementwise. We consider the simplified model where $\beta = (1, \ldots, 1)^T$. Now we think of the information $U_W(X)$ as a tensor

$$U_W(X) = \sigma'(f(W, X))^2 \nabla f(W, X)^{\otimes 2}.$$  

Then we have

$$\mathbb{E}U_W(X) = \mathbb{E}[\sigma'(f(W, X))^2(\tilde{\sigma}'(WX))^{\otimes 2}(X^{\otimes 2})^T].$$
and similarly,
\[ \mathbb{E}[v_W(X)U_W(X)] = \mathbb{E}[v_W(X)\sigma'(f(W,X))^2(\tilde{\sigma}'(W,X))^{\otimes 2}(X^{\otimes 2})^\top]. \]

**Shift invariance.** To characterize the efficiency gain, we assume the actions are circular shifts. Instead of computing \( \mathbb{E}\text{Cov}_G \nabla L_W(gX) \), we directly compute
\[
\mathbb{E}[U_W(X)](\Sigma_{\text{ERM}} - \Sigma_{a\text{ERM}})\mathbb{E}[U_W(X)] = \mathbb{E}
\left[
\left(\frac{v_W(X)\sigma'(f(W,X))^2}{\mathbb{E}_G[\sigma'(f(W,gX))]\nabla f(W,gX)}\right) \otimes^2 \right]
\times \left((\tilde{\sigma}'(W,X))^{\otimes 2}(X^{\otimes 2})^\top - (\tilde{\sigma}'(WC_X))^{\otimes 2}(C_X^{\otimes 2})^\top)\right].
\]
Assuming \( \tilde{\sigma}(x) = x^2/2 \), we have
\[
\mathbb{E}[U_W(X)](\Sigma_{\text{ERM}} - \Sigma_{a\text{ERM}})\mathbb{E}[U_W(X)] = W^{\otimes 2}\mathbb{E}
\left[
\left(v_W(X)\sigma'(f(W,X))^2\right)
\times \left((XX^\top)^{\otimes 2} - (C_XC_X^\top)^{\otimes 2}\right)\right].
\]

Similar to the regression case, the efficiency gain is governed by \((XX^\top)^{\otimes 2} - (C_XC_X^\top)^{\otimes 2}\). This gives an expression for the improvement due to augmentation, and it is unclear if it can be simplified further.

### 5.4 Linear regression

We study the linear regression problem in more detail. This is a special case of the exponential family model discussed before, but we can obtain more detailed results. Consider the linear model \( y = x^\top \beta + \varepsilon \) with loss function \( L(\beta, y, x) = (y - x^\top \beta)^2 \). We assume \( x \sim P_X, \varepsilon \sim P_\varepsilon \) and the two random variables are independent. We also assume \( P_\varepsilon \) has zero mean and its variance is \( \sigma^2 \).

We assume \( P_\varepsilon \) is a Gaussian measure and
\[
y \mid x \overset{d}{=} y \mid gx,
\]
for \( P_X \)-a.e. \( x \) and \( \mathbb{Q} \)-a.e. \( g \). This is saying that we have
\[
x^\top \beta = (gx)^\top \beta
\]
for \( P_X \)-a.e. \( x \) and \( \mathbb{Q} \)-a.e. \( g \). This is a set of linear constraints on the regression coefficient \( \beta \). For all \( x, g \) we get a linear constraint. Formally, supposing that \( x \) can take any value, we conclude that \( \beta \) is constrained to be in the invariant subspace of \( G \),
\[
I(G) = \{v : g^\top v = v, \forall g \in G\}.
\]
Letting \( d(G) = \dim I(G) \) be the dimension of the invariant space, this is a \( d(G) \)-dimensional linear constraint. If \( x \) can only take values in a smaller subset of \( \mathbb{R}^p \), then we get fewer constraints.

Suppose we observe i.i.d. data \( \{x_i, y_i\}_1^n \subseteq \mathbb{R}^p \times \mathbb{R} \). The augmented estimator is defined as
\[
\hat{\beta}_{aMLE} = \arg\min_{\beta} \sum_{i=1}^n \mathbb{E}_G(y_i - (gx_i)^\top \beta)^2.
\]
We consider the case where $G$ is linear. In this case, we can represent each $g \in G$ as a $p \times p$ invertible matrix. Then we have
\[
\hat{\beta}_{aMLE} = \arg \min_g \mathbb{E}_G \|y - X g^\top \beta\|^2_2
\]
\[
= \mathbb{E}_G \left( (X g^\top)^{-1} (X g^\top)^\top y \right)
\]
\[
= \mathbb{E}_G \left( g X^\top X g^\top - 1 g X^\top (X g^\top \beta + \varepsilon) \right)
\]
\[
= \beta + \mathbb{E}_G \left( g X^\top X g^\top - 1 g X^\top \varepsilon \right)
\]
\[
= \beta + \mathbb{E}_G \left( g^{-1} (X^\top X)^{-1} g X^\top \varepsilon \right)
\]
\[
= \beta + \mathbb{E}_G \left( g^{-1} (X^\top X)^{-1} X^\top \varepsilon \right)
\]
\[
= \beta + \mathbb{E}_G \left( g^{-1} (X^\top X)^{-1} X^\top \varepsilon \right)
\]

Let us denote $G := \mathbb{E}_G [g]$. Let $X = U D V^\top$ be a SVD of $X$, where $V \in \mathbb{R}^{p \times p}$ is unitary. Note that $\hat{\beta}_{aMLE}$ is unbiased, so its $\ell_2$ risk is
\[
r_{aMLE} = \sigma^2 \text{tr}(\text{Var}(\hat{\beta}_{aMLE})) = \sigma^2 \text{tr}(G (X^\top X)^{-1} G)
\]
\[
= \sigma^2 \text{tr}(G V D^{-2} V^\top G) = \sigma^2 \text{tr}(D^{-2} V^\top G G^\top V)
\]
\[
= \sigma^2 \sum_{j=1}^{p} d_j^{-2} e_j^\top G G^\top V e_j = \sigma^2 \sum_{j=1}^{p} d_j^{-2} \|G v_j\|^2_2,
\]
where $v_j \in \mathbb{R}^p$ is $j$-th eigenvector of $X^\top X$ and $d_j^2$ is $j$-th eigenvalue of $X^\top X$. As a comparison, the usual MLE is
\[
\hat{\beta}_{MLE} = (X^\top X)^{-1} X^\top y = \beta + (X^\top X)^{-1} X^\top \varepsilon,
\]
so its $\ell_2$ risk is
\[
r_{MLE} = \sigma^2 \text{tr}((X^\top X)^{-1}) = \sigma^2 \sum_{j=1}^{p} d_j^{-2}.
\]
So we get the following proposition:

**Proposition 5.2.** Assume $G$ is linear and $\sum_{j=1}^{p} d_j^{-2} \|G v_j\|^2_2 < \sum_{j=1}^{p} d_j^{-2}$. Then we have $r_{aMLE} < r_{MLE}$.

Furthermore, the constrained MLE is
\[
\hat{\beta}_{cMLE} = \arg \min_x \|y - X \beta\|^2_2
\]
\[
\text{s.t. } (g^\top - I_p) \beta = 0 \forall g \in G.
\]

Another way to see this is to realize that for $r_{aMLE} \leq r_{MLE}$ we need to show
\[
\text{tr}((X^\top X)^{-1} G G^\top) \leq \text{tr}((X^\top X)^{-1}).
\]
A sufficient condition is that, in the partial ordering of positive semidefinite matrices (also known as the Loewner order)
\[
GG^\top \leq I_p.
\]
This is equivalent to the claim that for all $v$ $\|\mathbb{E}_G g^\top v\|^2 \leq \|v\|^2$. However, by Jensen’s inequality, $\|\mathbb{E}_G g^\top v\|^2 \leq \mathbb{E}_G \|g^\top v\|^2$. Assuming $G$ is a subgroup of the orthogonal group $O(p)$, we have $\|g^\top v\|^2 = \|v\|^2$, hence we arrived to the following result.

**Proposition 5.3.** Assume $G$ is a subgroup of the orthogonal group. Then, for any design matrix we have $r_{aMLE} \leq r_{MLE}$.
**Permutation group.** Let us consider a special case, where \( G \) is the permutation group on \( \{1, 2, \ldots, p\} \). This group is clearly a subgroup of the orthogonal group, and hence augmentation decreases the risk. In this case, we can also get a closed-form expression for \( \hat{\beta}_{c,MLE} \). Note that invariance w.r.t. \( G \) implies that the true parameter is a multiple of the all ones vector: \( \beta = 1_p b \). So we have

\[
\hat{\beta}_{c,MLE} = 1_p \hat{b}, \quad \hat{b} = \arg \min \|y - X_1 p b\|_2^2.
\]

Solving the least-squares equation gives

\[
\hat{b} = \frac{1_p^\top X^\top y}{1_p^\top X^\top X 1_p}.
\]

The risk of estimating \( b \) is then \( \sigma^2 (1_p^\top X^\top X 1_p)^{-1} \), so that the risk of estimating \( \beta \) by \( 1_p \hat{b} \) is

\[
r_{c,MLE} = \sigma^2 p (1_p^\top X^\top X 1_p)^{-1}.
\]

For sake of comparison, we write.

\[
r_{a,MLE} = \frac{\sigma^2}{p^2} \text{tr}(1_p 1_p^\top (X^\top X)^{-1} 1_p 1_p^\top) = \frac{\sigma^2}{p} 1_p^\top (X^\top X)^{-1} 1_p,
\]

We then collect our result in the following proposition:

**Proposition 5.4.** If \( G \) is the permutation group over \( \{1, \ldots, p\} \), then we have

\[
r_{MLE} = \sigma^2 \text{tr}((X^\top X)^{-1}), \quad r_{a,MLE} = \sigma^2 p^{-1} 1_p^\top (X^\top X)^{-1} 1_p, \quad r_{c,MLE} = \sigma^2 p(1_p^\top X^\top X 1_p)^{-1}.
\]

Furthermore, if \( X^\top X = I \), we have

\[
r_{MLE} = p \sigma^2, \quad r_{a,MLE} = r_{c,MLE} = \sigma^2.
\]

The above proposition extends directly when \( G \) is the permutation group on a subset of \( \{1, \ldots, p\} \). There are several other subgroups of interest of the permutation group, including the group of cyclic permutations and the group that contains the identity and the operation that “flips” or reverses each vector.

We note briefly that the above results apply *mutatis mutandis* to logistic regression. There, the outcome \( Y \) is binary, and \( P(Y = 1 | X = x) = \sigma(x^\top \beta) \), where \( \sigma(z) = 1/(1 + \exp(-z)) \) is the sigmoid function. The invariance condition reduces to the same as for linear regression. We omit the details.

### 5.5 Cryo-EM and related problems

In this section, we describe several important problems in the biological and chemical sciences, and how data augmentation may be useful. Cryo-Electron Microscopy (Cryo-EM) is a revolutionary technique in structural biology, allowing us to determine the structure of molecules to an unprecedented resolution (e.g., Frank, 2006). The technique was awarded the Nobel Prize in Chemistry in 2017.

The data generated by Cryo-EM poses significant data analytic (mathematical, statistical, and computational) challenges (Singer, 2018). In particular, the data possesses several invariance properties that can be exploited to improve the accuracy of molecular structure determination. However, exploiting these invariance properties is highly nontrivial, because of the massive volume of the data, and due to the high levels of noise. In particular, exploiting the invariance is an active area of research (Kam, 1980; Frank, 2006; Zhao et al., 2016; Bandeira et al., 2017; Bendory et al., 2018). Classical and recent approaches involve mainly (1) latent variable models for the unknown symmetries, and (2) invariant feature approaches. Here we will explain the problem, and how data augmentation may help.

In the imaging process, many copies of the molecule of interest are frozen in a thin layer of ice, and then 2D images are taken via an electron beam. A 3D molecule is represented by an electron density map \( \phi : \mathbb{R}^3 \to \mathbb{R} \). Each molecule is randomly rotated, via a rotation that can be represented by a 3D orthogonal rotation matrix \( R_i \in O(3) \). Then we observe the noisy line integral

\[
Y_i = \int z \phi(R_i [x, y, z] \top) dz + \varepsilon_i.
\]
We observe several iid copies, and the goal is to estimate the density map $\hat{\phi}$. Clearly the model is invariant under rotations of $\phi$. Existing approaches mainly work by fitting statistical methods for latent variable models, such as the expectation maximization (EM) algorithm. Data augmentation is a different approach, where we add the data transformed according to the symmetries. It is interesting, but beyond our scope, to investigate if this can improve the estimation accuracy.

**Invariant denoising.** A related problem is invariant denoising, where we want to denoise images subject to an invariance of their distribution, say according to rotations (see e.g., Vonesch et al., 2015; Zhao et al., 2016, 2018). This area is well studied, and popular approaches rely on invariant features. It is known how to do it for rotations. However, capturing translation-invariance poses complications to the invariant features approach. In principle, data augmentation could be used as a more general approach.

**XFEL.** Another related technique, X-ray free electron lasers (XFEL), is a rapidly developing and increasingly popular experimental method for understanding the three-dimensional structure of molecules (e.g., Favre-Nicolin et al., 2015; Maia and Hajdu, 2016; Bergmann et al., 2017). Single molecule XFEL imaging collects two-dimensional diffraction patterns of single particles at random orientations. A key advantage is that XFEL uses extremely short femtosecond X-ray pulses, during which the molecule does not change its structure. On the other hand, we only capture one diffraction pattern per particle and the particle orientations are unknown, so it is challenging to reconstruct the 3D structure at a low signal-to-noise ratio. The images obtained are very noisy due to the low number of photons that are typical for single particles (Pande et al., 2015).

A promising approach for 3-D structure reconstruction is Kam’s method (Kam, 1977, 1980; Saldin et al., 2009), which requires estimating the covariance matrix of the noiseless 2-D images. This is extremely difficult due to low photon counts, and motivated prior work to develop improved methods for PCA and covariance estimation such as ePCA (Liu et al., 2018), as well as the steerable ePCA method Zhao et al. (2018) that builds in invariances. As above, it would be interesting to investigate if we can use data augmentation to as another approach for rotation-invariance.

### 5.6 Spherically invariant data

Here we discuss models for spherically invariant data, and how data augmentation may be used. See for instance Fisher et al. (1993) for more general models of spherical data. In the invariant model, the data $X \in \mathbb{R}^p$ is such that $X = OX$ for any orthogonal matrix $O$. One can see that the Euclidean norms $\|X\|$ are sufficient statistics. There are several problems of interest:

- Estimating the radial density. By taking the norms of the data, this reduces to estimating their 1D density.
- Estimating the marginal density $f$ of a single coordinate. Here it is less obvious how to exploit spherical invariance. However, data augmentation provides an approach.

A naive estimator for the marginal density is any density estimator applied to the first coordinates of the data, $X_1, \ldots, X_n$. Since $X_i \sim \text{iid} f$, we can use any estimator, $\hat{f}(X) = \hat{f}(X_1, \ldots, X_n)$ for instance a kernel density estimator. However, this is inefficient, because it does not use information in all coordinates.

In data augmentation we rotate our data uniformly, leading to

$$\hat{f}_a(X) = \int \hat{f}(gX)dQ(g) = \mathbb{E}_{O_1, \ldots, O_p \sim O(p)} f([O_1 X_1](1), \ldots, [O_p X_p](1)).$$

Note that if $O \sim O(p)$, then for any vector $x$, $[O x](1) = \|x\| Z(1)/\|Z\|$, where $Z \sim \mathcal{N}(0, I_p)$. Hence the expectation can be rewritten in terms of Gaussian integrals. It is also possible to write it as a 2-dimensional integral, in terms of $Z(1), \|Z(2 : p)\|^2$, which have independent normal and Chi-squared distributions. However, in general it may be hard to compute exactly.

When the density estimator decouples into a sum of terms over the datapoints, then this expression simplifies. This is the case for kernel density estimators: $\hat{f}(x) = (nh^p)^{-1} \sum_{i=1}^n k([x - x_i(1)]/h)$. More
generally, if \( \tilde{T}(x) = \sum_{i=1}^{n} T(x - x_i(1)) \), then we only need to calculate
\[
\tilde{T}(x) = \mathbb{E}_O T(x - [Oy](1)) = \mathbb{E}_{Z \sim \mathcal{N}(0, I_p)} T \left( x - \frac{\|y\|}{\|Z\|} Z(1) \right).
\]
This is significantly simpler than the previous expression. It can also be viewed as a form of convolution of a kernel with \( T \), which is already a kernel typically. Therefore, we have shown how data augmentation can be used to estimate the marginal density of coordinates for spherically uniform data.

5.7 Random effects models

Data augmentation may have applications to certain random effect models (Searle et al., 2009). Consider the one-way layout \( X_{ij} = \mu + A_i + B_{ij}, i = 1, \ldots, s, j = 1, \ldots, n_i \), where \( A_i \sim \mathcal{N}(0, \sigma_A^2), B_{ij} \sim \mathcal{N}(0, \sigma_B^2) \) independently. We want to estimate the global mean \( \mu \) and the variance components \( \sigma_A^2, \sigma_B^2 \). If the layout is unbalanced, that is the number of replications is not equal, this can be somewhat challenging. Two general approaches for estimation are the restricted maximum likelihood (REML), and minimum norm quadratic estimation (MINQUE) methods.

Here is how one may use data augmentation. Consider a simple estimator of \( \sigma_B^2 \) such as \( \hat{\sigma}_B^2 = s^{-1} \sum_{i=1}^{n} \mathbb{E}(X_{1i} - X_{2i})^2 / 2 \) (we assume that \( n_i \geq 2 \) for all \( i \)). This is a heuristic plug-in estimator, which is convenient to write down and compute in a closed form. It is also unbiased. However, it clearly does not use all samples, and therefore, it should be possible to improve it.

Now let us denote by \( X_i \) the block of \( i \)-th observations. These have a joint normal distribution \( X_i \sim \mathcal{N}(\mu 1_{n_i}, \sigma_A^2 1_{n_i} 1_{n_i}^\top + \sigma_B^2 I_{n_i}) \). The model is invariant under the operations
\[
X_i \rightarrow O_i X_i.
\]

For any orthogonal matrix \( O_i \) of size \( n_i \) for which \( O_i 1_{n_i} = 1_{n_i} \), i.e., a matrix that has the vector of all ones \( 1_{n_i} \) as an eigenvector. Let \( G_i \) be the group of such matrices. Then the overall model is invariant under the action of the direct product \( G_1 \times G_2 \times \ldots \times G_s \). Therefore, any estimator that is not invariant with respect to this group can be improved by data augmentation.

Going back to the estimator \( \hat{\sigma}_B^2 \), to find its augmented version, we need to compute the quantity \( \mathbb{E}([Ox]_1 - [Or]_2)^2 \), where \( x \in \mathbb{R}^k \) is fixed and \( O \) is uniformly random from the group of orthogonal matrices such that \( O 1_k = 1_k \). Write \( x = \pi 1_k + r \), where \( \pi \) is the mean of the entries of \( x \). Then \( Ox = \pi 1_k + Or \), and \( [Or]_j = \pi + [Or]_j \). Thus we need \( \mathbb{E}([Or]_1 - [Or]_2)^2 \). This can be done by using that \( Or \) is uniformly distributed on the \( k - 1 \) dimensional orthocomplement of the \( 1_k \) vector, and we omit the details.

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6 Appendix

6.1 Invariant MLE

Another perspective to exploit invariance is that of invariant representations. The natural question is, how can we work with invariant representations, and what are the limits of information we can extract from them?
Suppose therefore that in our model it is possible to choose a representation \( T(x) \) such that \((T(x),0_m) \in G \cdot x \) for all \( x \) (where \( 0_m \) is the zero vector with \( m \) entries). Thus, \( T \) chooses a representative from each orbit. This is equivalent to \((T(x),0_m) = g_0(x) \cdot x \), for some specific \( g_0(x) \in G \). Suppose \( T(\cdot),g(\cdot) \) satisfy sufficient regularity conditions, such as smoothness. For example, when \( G \) is the orthogonal rotation group \( O(d) \), we can take \( T(x) := \|x\|_2 \), and \( g \) any orthogonal rotation such that \( g_0(x) = (\|x\|_2,0_{d-1}) \).

How can we estimate the parameters \( \theta \) based on this representation? A natural approach is to construct the MLE based on the data \( T(X_1),\ldots,T(X_n) \). We can also construct invariant ERM using the same principle, but we will focus on MLE first. Let therefore \( Q_{\theta} \) be the induced distribution of \( T(X) \), when \( X \sim P_{\theta} \), and assume it has a density \( q_{\theta} \) with respect to Lebesgue measure on a potentially lower dimensional Euclidean subspace (say \( d' \) dimensional, where \( d \) is original dimension and \( m = d - d' \)). We can construct the invariant MLE (iMLE):

\[
\hat{\theta}_{\text{iMLE},n} = \arg \max_{\theta} \sum_{i \in [n]} \log q_{\theta}(T(X_i)).
\]

How does this compare to the previous approaches? It turns out that in general this is not better than the unaugmented MLE. Suppose that the group \( G \) is discrete. Then we have

\[
q_T(t) = \sum_{g \in G} p_X(g \cdot (t,0)) = |G| \cdot p_X((t,0)).
\]

Therefore, in this case the iMLE equals the MLE. Therefore, the invariant MLE does not actually gain anything over the usual MLE, and in particular augmented MLE is better.

6.2 Experiment details

Our experiment is standard: We train ResNet18 (He et al., 2016) on CIFAR10 for 200 epochs, based on the code of https://github.com/kuangliu/pytorch-cifar. We use the default settings from that code, including the SGD optimizer with a learning rate of 0.1, momentum 0.9, weight decay \( 5 \cdot 10^{-4} \), and batch size of 128. We train three models: (1) without data augmentation, (2) horizontally flipping the image with 0.5 probability, and (3) a composition of randomly cropping a 32 \times 32 portion of the image and random horizontal flip. We train both on the full CIFAR10 training data, as well as and a randomly chosen half of the training data. We do this to evaluate the behavior of data augmentation in the limited data regime, because there it may to lead to higher benefits.

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