Towards universal neural nets: Gibbs machines and ACE.

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Abstract

We study from a physics viewpoint a class of generative neural nets, *Gibbs machines*, designed for gradual learning. While including variational auto-encoders, they offer a broader universal platform for incrementally adding newly learned features, including physical symmetries. Their direct connection to statistical physics and information geometry is established. A variational Pythagorean theorem justifies invoking the exponential/Gibbs class of probabilities for creating brand new objects. Combining these nets with classifiers, gives rise to a brand of universal generative neural nets - stochastic auto-classifier-encoders (ACE). ACE have state-of-the-art performance in their class, both for classification and density estimation for the MNIST data set.

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1 Introduction.

1.1 Universality.

We buck the recent trend of building highly specialized neural nets by exploring nets which accomplish multiple tasks without compromising performance. An universal net can be tentatively described as one which, among other things: i) works for a variety of applications, i.e. visual recognition/reconstruction, speech recognition/reconstruction, natural language processing, etc; ii) performs various tasks: classification, generation, probability density estimation, etc; iii) is self-contained, i.e., does not use specialized external machine learning methods; iv) is biologically plausible.

1.2 Probabilistic and quantum viewpoint on generative nets.

The input of a neural net is typically a $P \times N$ data matrix $X$. Its row-vectors $\{x_\mu\}_{\mu=1}^P$ span the space of observations, its column-vectors $\{x_i\}_{i=1}^N$, where $1...N$ can for example enumerate the pixels on a screen, span the space of observables. The net is then asked to perform classification, estimation, generation, etc, tasks on it. In generative nets, this is accomplished by randomly generating $L$ latent observations $\{z^{(\kappa)}_\mu\}_{\kappa=1}^L$ for every observation $x_\mu$. This induced “uncertainty” of the $\mu$-th state is modeled by a model conditional density $p(z|x_\mu)$. It is the copy-cat, in imaginary time/space, of the (squared) wave function from quantum mechanics and fully describes the $\mu$-th conditional state $\{x_\mu, \{z^{(\kappa)}_\mu\}_{\kappa=1}^L\}$. In statistical mechanics parlance, the latents are fluctuating microscopic variables, while the macroscopic observables are obtained from them via some aggregation. In the absence of physical time, observations are thus interpreted as partial equilibria of independent small parts of the expanded (by a factor of $L$) original data set. Simply put, every visible observations is surrounded by a “cloud” of virtual observations. Creating a new original observation amounts to nothing more than sampling from that cloud.

The quality of the model conditional density, or more generally - the model joint density $p(z, x_\mu)$ - is judged by the “distance” from the implied marginal density $q(x) := \int p(x, z)dz$ to the empirical marginal density $r(x)$. This distance is called cross-entropy or negative log-likelihood:

$$- \log L(q|r) := \mathbb{E}_{r(x)}[- \log q(x)], \quad (1.1)$$

where $\mathbb{E}_{r(x)}[.]$ is an expectation with respect to $r()$. Its minimization is the ultimate goal.

1.3 Equilibrium setting. Gibbs machines.

The equilibrium i.e. small fluctuations viewpoint of statistical mechanics appears to have been originated by Einstein in a then-unpublished 1910 lecture [Einstein 2006]. He used an exponential model density $p^{\text{Exp}}$ in space and derived the Brownian diffusion i.e., Gaussian model density $p^{\text{G}}$ in space/time. They are special cases of a broad class of densities - Gibbs or exponential densities - which form the foundation of classic statistical mechanics. Gibbs densities are variational maximum-entropy densities and hence optimal for modeling equilibria. They also offer a platform for adding incrementally new macroscopic descriptive variables. [Landau and Lifshitz 1980], section 35.

We argue in sub-sections 2.6, 3.7 that Gibbs densities are also optimal for modeling fully-generative equilibria nets, and call those nets Gibbs machines. They were inspired by the first fully-generative nets - the variational auto-encoders (VAE [Kingma and Welling 2014], Rezende et al. 2014) - and employ the same upper bound for the cross-entropy target (1.1). Like their physics counterparts, Gibbs machines offer a platform for mimicking the gradual nature of learning: already learned symmetries in space/time symmetries, can be added incrementally and accelerate learning, sections 1.6, 2.3, 4.

1.4 Observation entropies

Unlike equilibrium statistical mechanics, human data is decidedly non-equilibrium in nature and exhibits large fluctuations and non-Gaussian behavior. Quantifying non-Gaussianity and “distance” from equilibrium is not easy when dealing with large number of observables $N$.
and observations \( P \). Luckily, there is a one-dimensional proxy for non-Gaussianity of a multi-dimensional data set: the non-Gaussianity of the negative Gaussian log-likelihoods \( \{- \log p^G(z_\mu)\}_{\mu} \). Here, \( - \log p^G(z_\mu) = \frac{1}{2} \langle z_\mu, C(z) \rangle^{-1} z_\mu + \text{const} \), with a multivariate Gaussian \( N_{N_{\text{lat}}} (0, C(z)) \) as model density and \( C(z) \) the empirical covariance.\(^{2}\)

In a bold and counter-intuitive re-read of Boltzmann’s statistical mechanics, Einstein interpreted the log-likelihoods \( \{ \log p^G(z_\mu) \}_{\mu} \) as observation entropies \(^{3}\) Ein- stein [2006]. We will denote the Einstein entropy \( S^E \) of an observation \( z_\mu \) by:

\[
S^E(z_\mu) := \log p^G(z_\mu) + \text{const} \geq 0. \tag{1.2}
\]

The sub-section [1.2] viewpoint of an observation, as a partial equilibrium of multiple virtual observations, fits right into Einstein’s paradigm: entropy is defined in a classical Boltzmann fashion, but on a cloud of virtual observations. The visible observation stands out as the one with a locally maximum entropy.

Observation entropies are central to modern theory of fluctuations \(^{4}\) Landau and Lifshitz [1980], chapter 12. They also have an elegant linear-algebraic incarnation in the singular value decomposition of the data matrix \( X \) (sub-section 5.1). In addition, their second moment \( \mathbb{E}_\mu \left[ \left( \log p^G(z_\mu) \right)^2 \right] \) is proportional to the multi-variate kurtosis, measuring the “fatness” of the probability density of \( \{ z_\mu \} \).

### 1.5 The equilibrium curse. Intricates.

Unfortunately, some of the key features of modern neural nets, like non-linear activation functions and dropout \(^{5}\) Srivastava et al. [2014], come at the high price of Gaussianizing the data set, i.e. lead to higher-entropy, less informative configurations. The right quantile-quantile (Q) plot in Figure 1 shows the Gaussianization effect of non-linearities and dropout for the MNIST data set \(^{6}\) LeCun et al. [1998]. Bounded non-linearities Gaussianize because they are compressive in nature and “straighten out” the unlikely (with small entropies) observations, which we refer to as intricates. Dropout Gaussianizes because it drops latent variables and thus decreases the kurtosis.

![Q-Q plots against a Gaussian of the density](image)

**Figure 1:** Q-Q plots against a Gaussian of the density of the negative log-likelihoods \( \{- \log p^G(z_\mu)\}_{\mu} \) of the 10000 MNIST test observations in layer 2 of a 5-layer standard feed-forward classifier net, see right branch of Figure 5 and Appendix A for implementation details. Layer sizes are 784-700-700-700-10. Learning rate = 0.0015, decay = 500 epochs, batch size = 10000. For the right plot, dropout is 0.2 in input layer and 0.5 in hidden layers. As an exception from the rules in Appendix A a tanh() activation function is used in the first hidden layer. **Left.** No dropout and no non-linearity: highly non-Gaussian. **Right.** With dropout and non-linearity: severely Gaussianized, especially for the intricates towards the right (see text).

It is precisely the intricates, which - because of their low entropy and extreme non-Gaussianity, see Figure 2 - are ideal candidates for “feature vectors” in classification tasks \(^{7}\) Hyvarinen et al. [2009], section 7.9, 7.10. Their conjugates are then the “receptive fields” or “feature detectors” \(^{8}\) - see open problem 1 in section 6. We show on the top (respectively, bottom) plot in Figure 3 the 30 least (respectively, most) likely images in MNIST, in ascending

\(^{2}\) If the latent observations \( \{ z_\mu \}_{\mu=1}^P \) come from an \( N_{N_{\text{lat}}} \)-dimensional Gaussian distribution, the density of these negative Gaussian log-likelihoods is proportional to the familiar \( F(N_{N_{\text{lat}}}, P - N_{N_{\text{lat}}}) \) density \(^{9}\) Mardia et al. [1979], sections 1.8, 3.5. For the typical case \( P - N_{N_{\text{lat}}} \to \infty \), it is proportional to the chi-squared density \( \chi^2_{N_{N_{\text{lat}}}}(\cdot) \), which in turn converges to a rescaled Gaussian \( \mathcal{N}(0,1) \), as \( N_{N_{\text{lat}}} \to \infty \).

\(^{3}\) In order for the negative logs to be thought of as entropies, a large positive constant is added. It should be clear from the context, but we nevertheless use for clarity a superscript, to distinguish the Einstein entropy \( S^E(\cdot) \) of an observations, from the standard Boltzmann entropy \( S(\cdot) \) of a probability density, introduced in sub-section [2.1].

\(^{4}\) Recall that, for a given row-vector observation \( x_\mu \), its conjugate is \( \tilde{x}_\mu = x_\mu C^{-1} \), where \( C \) is the covariance matrix. Up to a constant, the Gaussian negative log-likelihood is thus the inner product of an observation and its conjugate, in the standard Euclidean metric:

\[
- \log p^G(x_\mu) = \frac{1}{2} \langle x_\mu, x_\mu \rangle = \frac{1}{2} \langle x_\mu, \tilde{x}_\mu \rangle.
\]
order of their entropy $S^E$, from the class corresponding to the digit 8.

Figure 2: **Left.** The first 5000 MNIST training images, projected on three of the least likely, i.e. most intricate conjugate images, ranked #3, #4, #6 in ascending order of Einstein entropy $S^E(x_{ij})$. This is a highly non-Gaussian 3-dimensional distribution. **Right.** The same MNIST images, projected on the three most likely conjugate images, ranked #4998, #4999, #5000 in Einstein entropy. Much more Gaussian-looking.

Figure 3: **Top.** The 30 lowest-entropy MNIST training images, using the Einstein entropy $S^E(z_{ij})$, from the class corresponding to the digit 8. They are quite intricate indeed. **Bottom.** The 30 highest-entropy MNIST training images from the same class. Much more vanilla-looking.

1.6 Symmetries in the latent manifold.

When the dimensionality $N_{lat}$ of the ACE latent layer is low, traversing the latent dimension in some uniform fashion describes the latent manifold for a given class. Figure 4 shows the dominant dimension for each of the 10 classes in MNIST. This so-called manifold learning by modern feed-forward nets was pioneered by the contractive auto-encoders (CAE) [Rifai et al., 2012]. A symmetry in our context is, loosely speaking, a one-dimensional parametric transformation, which leaves the cross-entropy unchanged. In probabilistic terms, this is equivalent to the existence of a one-parametric density, from which “symmetric” observations are sampled, see (1.3) below. Nets currently learn symmetries from the training data, after it is artificially augmented, e.g. by adding rotated, translated, rescaled, etc, images, in the case of visual recognition. But once a symmetry is learned, it does not make sense to re-learn it for every new data set.

Figure 4: Dominant dimension for each of MNIST ten classes, with each row corresponding to a separate class. While rotational symmetry dominates most classes, size i.e. scaling symmetry, clearly dominates the class of digit 5. The net is an ACE in creative regime as in sub-section 3.3 with an equally spaced deterministic grid in the latent layer $\{-6 \leq \sigma \leq 6\}$. Layer sizes 784-700-(1x10)-(700x10)-(784x10) for the AE branch and 784-700-700-700-10 for the C branch, Figure 5 and Appendix A, learning rate $= 0.0002$, decay $= 500$ epochs, batch size $= 1000$.

We hence propose the reverse approach: add the symmetry explicitly to the latent layer, alongside its Noether invariant, Gelfand and Fomin [1963]. Take for example translational symmetries in a two-dimensional system with coordinates $(z^{(h)}, z^{(v)}) \in \mathbb{R}^2$. They imply the conservation of the horizontal and vertical momenta $(-ih\partial/\partial z^{(h)}, -ih\partial/\partial z^{(v)}) = (p^{(h)}, p^{(v)}) \in \mathbb{R}^2$ and a quantum mechanical wave function $\sim e^{\pm (p^{(h)}(z^{(h)} - h) + p^{(v)}(z^{(v)} - v))}$, where $(h, v)$ are offsets, Landau and Lifshitz [1977], section 15. After switching
to imaginary time SPACE in sub-section 1.2 and setting $h = 1$, the corresponding conditional model density for a given observation/state $\mu$ is:

$$p(z|x_\mu) \sim e^{-2p^{(h)}|z^{(h)} - h_\mu| - 2p^{(v)}|z^{(v)} - v_\mu|},$$

(1.3)
i.e. a two-dimensional Laplacian which fits in the Gibbs machine paradigm (2.7). We demonstrate in section 4 how to build-in translational, scaling and rotational symmetry in a net, by computing the symmetry statistics like $\{h_\mu, v_\mu\}$ explicitly and estimating the invariants with the rest of the net parameters. In general, they have to be refined via an optimization, as e.g. in Jadeberg et al. [2015]. For more details, see Georgiev [2015b].

1.7 ACE.

1.7.1 Non-generative ACE.

In order to preserve the non-Gaussianity of the data, and improve performance significantly along the way, we will combine classifiers with auto-encoders - hence the name auto-classifier-encoder (ACE). Auto-encoders have a reconstruction error in their cross-entropy optimization target and thus force the net to be more faithful to the raw data. ACE simultaneously classifies and reconstructs, assuming an independence between the two, and hence additivity of the respective cross-entropies:

$$-\log L_{ACE} = -\log L_{AE} - \log L_{CE}.$$  

(1.4)

In its first - non-generative - installment, ACE can do with a standard classifier and a shallow auto-encoder in the dual space of observations. It still beats handily the peers in its class, Figure 8, right.

1.7.2 Non-Gaussian densities.

In real-life data sets, the number of observations $P \to \infty$, while the dimension of observables $N$ is fixed. An

\[ {\text{universal net will hence tend to work better when the dimension of latent layers $N_{\text{lat}} \geq N$, i.e. have the so-called overcomplete representation [Coates et al. 2011]. When $N_{\text{lat}} >> N$, for any given $N$-dimensional observation $x_\mu$, only a small number of latents $\{z_{\mu j}\}_{j=1}^{N_{\text{lat}}}$ deviate significantly from zero. For these sparse representations, sampling from high-entropy Gaussian-like densities, as on the right plot of Figure 2, is flawed. Sampling instead from “fat-tail” densities offers a significant performance improvement for MNIST, Figure 9, right. As in mathematical finance, stochastic volatility and jumps are arguably the first natural source of non-Gaussianity, and are almost fully-tractable. The q-Gibbs machines offer another venue, sub-section 2.3.}}

1.7.3 Generative ACE.

An even greater issue for current nets is the spontaneous “clumping” or clusterization which is prevalent in real-life data sets. Statistical mechanics deals with it by introducing higher-hierarchy densities which are conditional on low-hierarchy densities. The Fermi density discussed in sub-section 3.1 is an example of a higher-hierarchy density, built on top of the Boltzmann density, subject to additional constraints Landau and Lifshitz [1980], section 53. Clusterization aggregates the low-hierarchy partial equilibria - the observations - into higher-hierarchy partial equilibria - clusters, sub-section 1.2.

To mimic this universal phenomenon, in its second, generative, installment, ACE combines a classifier and a generative auto-encoder in the same space of observables, in a brand of an auto-encoder supervision, Figure 5. ACE generalizes the classic idea of using separate decoders for separate classes, Hinton et al. [1995]. In training, the conditional latent density $p(z|x_\mu, \epsilon_\mu)$ from sub-section 1.2 is generalized to $p(z|x_\mu, \epsilon_\mu)$, where $\epsilon_\mu$ is the class or label of the $\mu$-th observation. Since, of course, classification labels can not be used on the testing set, the sampling during testing is from a mixture of densities, with class probabilities supplied by the classifier (hence the dashed line in Figure 5). Mixture densities in the posterior were also used in Kingma et al. [2014], albeit in a different architecture. The ACE is universal in the sense of subsection 1.4 and achieves state-of-the-art performance, both as a classifier and a density estimator, Figure 9. For its relation with information geometry, see open problem 6 in section...
2 Theoretical background.

2.1 Definitions.

For discrete data, our minimization target - the cross-entropy \( L_{	ext{cross}} \) - can be decomposed as the sum:

\[
- \log L_{\text{cross}} = S(r) + D(r||q),
\]

(2.1)

of the Kullback-Leibler divergence \( D(r||q) \) between empirical \( r() \) and model \( q() \) densities:

\[
D(r||q) := E_{r(x)}[\log r(x) - \log q(x)],
\]

(2.2)

and the standard Boltzmann entropy \( S(r) \) of \( r() \):

\[
S(r) := E_{r(x)}[-\log r(x)],
\]

(2.3)

\( S(.) \neq S^E(.) \). Because the entropy \( S(r) \) of \( r() \) does not depend on our model distribution \( q() \), the minimization of the cross-entropy is equivalent to minimizing the Kullback-Leibler divergence \( D(r||q) \). It is common in statistical physics, see e.g. [Naudts 2010], to formally consider \(-D(r||q)\) as a generalized entropy \( S_q(r) \), for the case of a non-trivial base measure \( q() \) - see (2.20) below.

As discussed in sub-section 1.2, the latents \( \{z\} \) in generative nets are sampled from a closed-form conditional model density \( p(z|x) \). The latents are of course not given a priori, so the joint empirical density is:

\[
r(x,z) = \frac{1}{P} \sum_{\mu} \delta(x-x_{\mu})p(z|x_{\mu}),
\]

(2.4)

with corresponding marginal empirical densities \( r(x) = \frac{1}{P} \sum_{\mu} \delta(x-x_{\mu}) \) and \( r(z) = \frac{1}{Z} \sum_{\mu} p(z|x_{\mu}) \) [Kulhavy 1996, section 2.3; Cover and Thomas 2006, problem 3.12]. Hence, the cross-entropy of \( q(x) := \int p(x,z)dz = p(x,z)/p(z|x) \) is an arithmetic average across observations \(-L(r||q) = -\frac{1}{P} \sum_{\mu} \log q(x_{\mu}) \). From the Bayes identity, we have for our optimization target \(-L_{\text{cross}} \) in

\[\text{Back-propagation of main (\(-\log \mathcal{L}_{\text{ACE}}\)) and reg-\text{constraints}},\]

\[\log \mathcal{L}_{\text{ACE}} = -\log \mathcal{L}_{\text{AE}} - \log \mathcal{L}_{\text{C}}\]

6
terms of the joint density:

\[- \log L(r || q) := \mathbb{E}_r(p(x))[- \log q(x)] = \mathbb{E}_r(x, z)[- \log p(x, z)] + \mathbb{E}_r(x, z)[\log p(z|x)]. \tag{2.5}\]

From the explicit form of \( r(x, z) \), for the \( \mu \)-th observation:

\[- \log q(x_{\mu}) = \mathcal{D}(p(z|x_{\mu})|p(x_{\mu}, z)) = \mathbb{E}_{p(x|x_{\mu})}[- \log p(x_{\mu}, z)] - S(p(z|x_{\mu})), \tag{2.6}\]

where \( S(p(z|x_{\mu})) = \mathbb{E}_{p(z|x_{\mu})}[- \log p(z|x_{\mu})] \) is the Boltzmann entropy of the model distribution, conditional on a given observation \( x_{\mu} \). If we sample the latent observables only once per observation, as commonly done, the right-hand side reduces to \(- \log p(x_{\mu}, z_{\mu}) + \log p(z_{\mu}|x_{\mu}) \).

### 2.2 Conditional independence.

The hidden/latent observables \( z = \{z_j\}_{j=1}^{N_{lat}} \) are conditionally independent if, for a given observation \( x_{\mu} \), one has \( p(z|x_{\mu}) = \prod_{j=1}^{N_{lat}} p(z_j|x_{\mu}) \). From the independence bound of the Boltzmann entropy \( S(p(z|x_{\mu})) \leq \sum_{j=1}^{N_{lat}} S(p(z_j|x_{\mu})) \), we see that conditional independence minimizes the negative entropy term on the right-hand side of (2.6). Everything else being equal, conditional independence is hence optimal for nets.

### 2.3 Exponential/Gibbs class of densities.

There is a broad class of probability density families - Gibbs a.k.a. canonical or exponential families - which dominate the choices of model densities, both in physics and neural nets. This class includes a sufficiently large density families: Gaussian, Bernoulli, exponential, gamma, etc. Their general closed form is:

\[ p(\lambda(z)) = \frac{p(z)}{Z} e^{-\sum_{j=1}^{N_{lat}} \lambda_j \mathcal{M}_j(z)}, \tag{2.7}\]

where \( p(z) \) is an arbitrary base or prior density, \( \lambda = \{\lambda_j\} \) are Lagrange multipliers a.k.a. natural parameters, \( \mathcal{M}_j(z) \) are so-called sufficient statistics, and \( Z = Z(\lambda) \) is the normalizing partition function. Knowing \( Z \) is equivalent to knowing the free energy \( F(\lambda) = -\log Z(\lambda) \), which allows to re-write (2.7) as:

\[ p_\lambda(z) = p(z)e^{\sum_{j=1}^{N_{lat}} \lambda_j \mathcal{M}_j(z)} = p(z)e^{F(\lambda) - \lambda \cdot \mathcal{M}(z)}, \tag{2.8}\]

where \( \lambda \cdot \mathcal{M} \) is the scalar product of the vectors \( \lambda = \{\lambda_j\} \) and \( \mathcal{M} = \{\mathcal{M}_j\} \).

### 2.4 Macroscopic quantities.

In physics, the expectations of the sufficient statistics \( m \) form a complete set of macroscopic a.k.a. thermodynamic quantities or state variables like energy, momenta, number of particles, etc, fully describing the \( \mu \)-th conditional state, see subsection 1.2, see Landau and Lifshitz [1980], sections 28, 34, 35, 110. In neural nets, the sufficient statistics are typically monomials like \( M_1(z) = z, M_2(z) = z^2, \) etc, whose expectations form a vector of moments. As proposed in sub-section 1.6, one can add them to the list the symmetry statistics, see section 3 for details. From the definition of free energy, one derives immediately that it is a generative function of the expectations \( m \):

\[ \frac{\partial F(\lambda)}{\partial \lambda} = m(\lambda), \tag{2.9}\]

and, more generally, of their higher n-th moments:

\[ \frac{\partial^{-1} F(\lambda)}{\partial \lambda_1 \partial \lambda_2 \ldots \partial \lambda_k} = (-1)^{n+1} \mathbb{E}_{p(\lambda)}[M_1(z)M_2(z)\ldots M_k(z)]. \tag{2.10}\]

### 2.5 Variational Pythagorean theorem.

The exponential/Gibbs class of families is special because it is the variational maximum entropy class: when the base density \( p() \) is trivial, it is the unique functional form which maximizes the Boltzmann entropy \( S(f) \) across the universe \( \{f(z)\} \) of all densities with given macroscopic quantities \( m = \mathbb{E}_f[\mathcal{M}(z)] \), see Cover and Thomas [2006] chapter 12. The natural parameters \( \lambda = \lambda(m) \) are computed so as to satisfy these constraints. They are Lagrange constraints multipliers in the variational calculus derivation of the maximum entropy property.
The Gibbs class is special in even stronger sense: it is a minimum divergence class. For an arbitrary base density \( p(z) \), the Kullback-Leibler divergence \( \mathcal{D}(p_\lambda(z)||p(z)) \) minimizes the divergence \( \mathcal{D}(f(z)||p(z)) \) across the universe \( \{f(z)\} \) of all densities with given macroscopic quantities \( m = E_f[M(z)] \). This follows from the variational Pythagorean theorem. Figure [Chentsov 1968]. Kulhavy [1996], section 3.3:

\[
\mathcal{D}(f(z)||p(z)) = \mathcal{D}(f(z)||p_\lambda(z)) + \mathcal{D}(p_\lambda(z)||p(z)) \\
\geq \mathcal{D}(p_\lambda(z)||p(z)). \tag{2.11}
\]

![Figure 6: A naive visualization of the probabilistic (variational) Pythagorean theorem from (2.11).](image)

### 2.6 Generative error.

As we will see in sub-section 2.7 minimizing the divergence \( \mathcal{D}(f(z)||p(z)) \) across an unknown a priori family of conditional distributions \( p(z|x_\mu) = f(z) \), is crucial for the quality of a generative net. The smaller this divergence, the more likely are the sampled from \( p(z) \) newly created objects to resemble the training set. The minimum divergence property (2.11) implies that we are always better off choosing \( p(z|x_\mu) \) from a Gibbs class, as in (2.13), hence the name Gibbs machines. We will refer to the minimum divergence \( \mathcal{D}(p(z|x_\mu)||p(z)) \) as generative error:

\[
\mathcal{D}^{gen}(m(x_\mu)) := \mathcal{D}(p(z|x_\mu)||p(z)) \geq 0. \tag{2.12}
\]

The lack of explicit dependence on the natural parameters \( \lambda \) on the left is because \( \mathcal{D}^{gen} \) depends on them only indirectly, via the macroscopic quantities \( m = m(\lambda) \) (see sub-section 2.9).

### 2.7 Conditional latent densities.

For a given observation \( x_\mu \), choosing a conditional latent density from the Gibbs type (2.3) is equivalent to:

\[
p(z|x_\mu) := p(z)e^{F^{gen}(x_\mu, \lambda) - \lambda M(z)}, \tag{2.13}
\]

where the superscript \( 'gen' \) is short for generative. We will see shortly that the free energy \( F^{gen} \) and the negative generative error \( -\mathcal{D}^{gen} \) from the previous sub-section are concave conjugates, hence the shared superscript. In practice, in order for \( p(z|x_\mu) \) to be tractable, \( p(z) \) has to be from a specific parametric family within the Gibbs class: then both \( p(z) \) and \( p(z|x_\mu) \) will be tractable and in the same family, e.g. Gaussian, exponential, etc.

Except for the symmetry statistics introduced in sections 1.6.4 the macroscopic quantities \( m(x_\mu) = E_{p(z|x_\mu)}[M(z)] \) for the \( \mu \)-th quantum state are free parameters. Together with the the symmetry statistics, they can be thought of as quantum numbers distinguishing the observations, a.k.a. partial equilibrium states, from one another, in the spirit of quantum statistics [Landau and Lifshitz 1980] section 5, see sub-section 1.2 here. These quantum numbers are added to the rest of the free net parameters, to be optimized by standard methods, like back-propagation/ stochastic gradient descent, etc.

### 2.8 Boltzmann-Gibbs thermodynamic identity.

The identities relating various macroscopic (thermodynamic) quantities are referred to in statistical physics as thermodynamic identities. Recall that the classic Boltzmann-Gibbs distribution is a special case of the exponential/Gibbs distribution (2.8), with a trivial base density \( p() \), and only one sufficient statistics - the microscopic energy or Hamiltonian \( H() \):

\[
p_{BG}(z|x_\mu) = e^{F(x_\mu) - \beta H(x_\mu, z)}, \tag{2.14}
\]

where \( \beta := \frac{1}{T} \) is the inverse temperature and the only natural parameter. Taking logs and expectations w.r.t. \( p_{BG}(z|x_\mu) \), one gets the classic thermodynamic identity for the free energy \( F^{BG} = F^{BG}(x_\mu, \beta) \) and entropy \( S(p_{BG}(z|x_\mu)) \):

\[
F^{BG}(\beta) = \beta U^{BG}(\beta) - S(U^{BG}(\beta)), \tag{2.15}
\]
where the only macroscopic quantity - the energy $U^{BG}$ - is the expectation $U^{BG} := \mathbb{E}_{p^{BG}(\mathbf{x}_n)}[\mathcal{H}(\mathbf{x}_n, \mathbf{z})]$. The entropy $S$ depends on $\beta$ only indirectly, via the energy i.e. $S = S(U^{BG}(\beta))$.

The increase of free energy has the physics interpretation of work needed to be done by the outside environment, in order to increase the macroscopic quantity of the system, i.e. the energy in this case. The negative sign in (2.15) confirms the intuition that, for the same increase of internal energy $U^{BG}$, less ordered systems need less work from the outside.

2.9 Generative thermodynamic identity.

As mentioned in sub-section 2.1, in a more general context like (2.13), the negative generative error $-\mathcal{D}^{gen}(\mathbf{m})$ plays the role of generalized entropy $S_p(p(z|x_n))$, with base measure $p(z)$. As is standard in statistical mechanics, it can be shown (Kulhavý [1996], Chapter 3) that $-\mathcal{D}^{gen}(\mathbf{m})$ is a concise function, expressible via the Legendre transform of its conjugate - the generative free energy $F^{gen}(\lambda)$:

$$-\mathcal{D}^{gen}(\mathbf{m}) = \min_{\lambda} \{ \lambda \cdot \mathbf{m} - F^{gen}(\lambda) \}, \quad (2.16)$$

or, equivalently,

$$\mathcal{D}^{gen}(\mathbf{m}) = \max_{\lambda} \{ -\lambda \cdot \mathbf{m} + F^{gen}(\lambda) \}, \quad (2.17)$$

where $\lambda \cdot \mathbf{m}$ is a scalar product of the vectors $\lambda$ and $\mathbf{m}$ and $\lambda$ is allowed to run free. Note that, while the variational Pythagorean theorem establishes the minimum property of $\mathcal{D}^{gen}$ as a functional $\mathcal{D}^{gen}(f||p)$ over the space of functions $\{f(z)\}$, $\mathcal{D}^{gen}$ is a maximum when viewed as an explicit function $\mathcal{D}^{gen}(\mathbf{m}, \lambda)$ of both the macroscopic quantities $\mathbf{m}$ and the natural parameters $\lambda$. Equivalently,

$$F^{gen}(\lambda) = \min_{\mathbf{m}} \{ \lambda \cdot \mathbf{m} + \mathcal{D}^{gen}(\mathbf{m}) \}, \quad (2.18)$$

where $\mathbf{m}$ is allowed to run freely. At the optimal point ("equilibrium") $\mathbf{m}^{gen}$, this implies the dual identity of (2.9):

$$- \frac{\partial \mathcal{D}^{gen}(\mathbf{m})}{\partial \mathbf{m}} \bigg|_{\mathbf{m} = \mathbf{m}^{gen}} =: \lambda^{gen}(\mathbf{m}^{gen}). \quad (2.19)$$

Similarly to (2.9), the derivative on the left-hand side defines the function $\lambda^{gen} = \lambda^{gen}(\mathbf{m})$ as a function of $\mathbf{m}$ everywhere. While generative free energy was defined in (2.18) for every $\lambda$, unless the function in (2.19) is invertible, its image is only a subset of the full space of natural parameters $\lambda$. Assuming such invertibility, the generalization of (2.13) is:

$$\mathcal{F}^{gen}(\lambda) = \mathbf{m}^{gen}(\lambda) + \mathcal{D}^{gen}(\mathbf{m}^{gen}(\lambda)), \quad (2.20)$$

where we skipped for brevity the dependence on $x_n$. Counter to classic thermodynamics (2.15), we have a plus sign? The two factors comprising the divergence $\mathcal{D}^{gen}([\lambda])$, clearly work against each other. On the one hand, the negative entropy term $-S(p(z|x_n)) \leq 0$ reduces free energy as usual: less ordered systems take less work to create. On the other hand, when the system resides in an infinitely-large "thermostat" of non-trivial density $p(z)$, the cross-entropy term $\mathbb{E}_{p(z|x_n)}[-\log p(z)] \geq 0$, increases the free energy back up. It measures the amount of work it takes to counter the thermostat’s influence.

The chain rule and (2.9), (2.19), give in addition the indirect dependence of $\mathcal{D}^{gen}$ on the natural parameters $\lambda$:

$$\frac{\partial \mathcal{D}^{gen}(\mathbf{m}(\lambda))}{\partial \lambda} = -\lambda \cdot \frac{\partial \mathbf{m}(\lambda)}{\partial \lambda} = -\lambda \cdot \frac{\partial^2 F^{gen}(\lambda)}{\partial \lambda \partial \lambda}. \quad (2.21)$$

From (2.10), this derivative is conveniently expressed in terms of the matrix of second moments of the sufficient statistics:

$$\frac{\partial \mathcal{D}^{gen}(\mathbf{m}(\lambda))}{\partial \lambda} = \lambda \cdot \mathbb{E}_{p(z|x_n)}[\mathcal{M}(z)\mathcal{M}(z)]. \quad (2.22)$$

2.10 q-Gibbs densities.

Gibbs densities are only a special case (for $q = 1$) of the broad class of q-Gibbs (or q-exponential) densities. The corresponding nonextensive statistical mechanics [Tsallis [2009], describes more adequately long-range-interacting many-body systems like typical human-generated data sets. By virtue of replacing the exponential with a q-exponential, log with q-log and defining a respective q-entropy, most of the formalism of classic thermodynamics has been generalized. Many of the properties of the exponential class remain true for the q-exponential class.
3 Application to generative neural nets.

A fully-generative net creates original observations by sampling from an unconditional model density \( p(z) \), unencumbered by any observations \( \{x_j\} \). Perturbative nets on the other hand, do not contain an unconditional model density \( p(z) \). They rely instead on an initial observation \( x_\mu \), a conditional density \( p(z|x_\mu) \), and the decomposition (2.6) for parameter estimation.

3.1 Perturbative nets.

The most successful family of perturbative nets to date have been the Boltzmann machines Smolensky [1986] and their multiple re-incarnations. Assuming completeness have been the dominant universal nets: They perform well both as classifiers Srivastava et al. [2014] and probability density estimators Salakhutdinov and Murray [2008].

3.2 Reconstruction error.

A neural net is said to have reconstruction capabilities, if it has a decoder, which for a given latent \( z \), can assign a reconstruction density \( p^{rec}(x_\mu|z) \) of an observation \( x_\mu \). Following standard procedure, the reconstruction error is the usual cross-entropy (1.1) of this reconstruction density and the empirical density (2.4):

\[
- \log L^{rec}(x_\mu) := \mathbb{E}_{p(x|x_\mu)}[- \log p^{rec}(x_\mu|z)] \geq 0. \tag{3.1}
\]

Reconstruction densities are typically from the exponential/Gibbs class - Bernoulli, Gaussian, etc - with unity covariance matrix, and a trivial base density \( p() \). But the key reconstruction macroscopic quantity - the expectation \( \mathbf{m}^{rec}(x_\mu) = \mathbb{E}_{p(x|x_\mu)}[x_\mu] \) - is generally an intractable function of \( z \), given by the net decoder.

The cross-entropy \( - \log L^{rec} \) depends on the generative natural parameters only via the expectation density \( p(z|x_\mu) \), and its derivatives are from (3.1):

\[
- \frac{\partial \log L^{rec}(\mathbf{m}(\lambda))}{\partial \lambda} = \mathbb{E}_{p(x|x_\mu)}[\mathcal{M}(z) \log p^{rec}(x_\mu|z)]. \tag{3.2}
\]

3.3 Fully-generative nets. Regimes.

We will distinguish two separate regimes of operation of a fully-generative net:

1. non-creative regime: This is the common regime for net training, validation or testing. Latent observables are sampled from a closed-form model conditional density \( p(z|x) \), as in sub-section 2.7 with observations \( \{x_j\} \) attached to the net. A closed-form reconstruction model density \( p^{rec}(x|z) \), as in sub-section 3.2 is also chosen.

2. creative regime: The net has been trained and latent observables \( z = \{z_j\}_{j=1}^{N_{out}} \) are sampled from a closed-form model density \( p(z) \), unencumbered by observations \( \{x_j\} \). The same reconstruction density \( p^{rec}(x|z) \) as in the non-creative regime is used.

The joint density is chosen to be:

\[
p(x, z) := p(z)p^{rec}(x|z). \tag{3.3}
\]

The empirical densities are the same as in sub-section 2.1.
3.4 Variational error.

The implied marginal density \( q(x) := \int p(x,z)dz \) and the implied conditional density \( q(z|x) = \frac{p(x,z)}{q(x)} \) are generally intractable in fully generative nets. Moreover, the implied conditional \( q(z|x) \) is of course different than our chosen \textit{a priori} \( p(z|x) \) in the non-creative regime. For a given observation \( x_m \), the divergence between the two is called variational error:

\[
D^{\text{var}}(x_m) = D(p(z|x_m)||q(z|x_m)) \geq 0. \tag{3.4}
\]

Its optimization is the subject of the so-called fixed-form variational Bayes analysis Saul and Jordan [1995]. We will discuss its estimation in sub-section 3.8, see also open problem 7, section 6.

3.5 Cross-entropy decomposition.

Following standard procedure, our training minimization target is the cross-entropy (1.1) between the marginal densities \( D = \sum \log \frac{p(x)}{q(x)} \). Expanding the joint density (3.3) in both Bayesian directions, one can decompose in terms of the implied conditional \( q(z|x_m) \) as follows:

\[
- \log \mathcal{L}(r||q) := \mathbb{E}_{r(z)}[- \log p(z)] + \\
\quad + \mathbb{E}_{r(x,z)}[- \log p^{\text{rec}}(x|z)] + \mathbb{E}_{r(x,z)}[\log q(z|x)] . \tag{3.5}
\]

From the explicit form (2.4) of \( r(x,z) \), for the \( \mu \)-th observation \( x_m \):

\[
- \log q(x_m) = \mathbb{E}_{p(z|x_m)}[- \log p(z)] + \\
\quad + \mathbb{E}_{p(z|x_m)}[- \log p^{\text{rec}}(x_m|z)] + \mathbb{E}_{p(z|x_m)}[\log q(z|x_m)] . \tag{3.6}
\]

Subtracting \( S(p(z|x_m)) \) from the first term and adding it to the third, and using the definitions (2.12) of generative error \( D^{\text{gen}} \), (3.1) of reconstruction error \( - \log L^{\text{rec}} \) and (3.4) of variational error \( D^{\text{var}} \), the final expression for our minimization target is:

\[
- \log q(x_m) = D^{\text{gen}}(x_m) - \log L^{\text{rec}}(x_m) - D^{\text{var}}(x_m). \tag{3.7}
\]

Let us highlight the essence and computability of each of the three components:

1. \( D^{\text{gen}} \geq 0 \): the generative error (2.12) is the divergence between the generative densities in the non-creative and creative regimes. Minimizing it ensures the general similarity of objects generated in the two regimes. It can be interpreted as the hypotenuse in the variational Pythagorean theorem (2.11) and is computable in closed form for many Gibbs/exponential densities.

2. \(- \log L^{\text{rec}} \geq 0 \): the reconstruction error (3.1) measures the negative likelihood of getting \( x_m \) back, after the transformations and randomness inside the net. It can be computed by any net endowed with a decoder via standard Monte Carlo averaging, as traditional auto-encoders do. Importantly for training, in order to compute gradients with respect to the generative macroscopic quantities \( D^{\text{gen}} \), a change of variable is needed, replacing sampling from \( p(z|x_m) \) by sampling from \( p(z) \). Such transformations exists for many of the exponential/Gibbs probability families Kingma and Welling [2014].

3. \( D^{\text{var}} \geq 0 \): the variational error (3.4) measures the divergence between our chosen functional form \( p(z|x_m) \) for latent density and the implied by the net latent density \( q(z|x_m) \). Due to the intractability of \( q(z|x_m) \), the variational error has to be computed numerically via Monte Carlo methods, see sub-section 3.8 and open problem 7, section 6.

3.6 Cross-entropy upper bound.

Dropping the variational error in (3.7) yields an upper bound \( B() \) for the cross-entropy\(^8\):

\[
B(x_m) := D^{\text{gen}}(x_m) - \log L^{\text{rec}}(x_m) = \\
\quad = D(p(z|x_m)||p(x_m,z)). \tag{3.8}
\]

While the last expression is formally equivalent to the general expression (2.6) for \(- \log q(x_m) \), the density \( p(z|x_m) \) in (2.6) is the correct conditional density of the joint density \( p(x_m,z) \), while \( p(z|x_m) \) here is merely an approximation to the implied conditional \( q(z|x_m) \).

From (2.22) and (3.2), the derivative of the upper bound

\(^8\)This is an expanded version of the textbook \textit{variational inequality} Cover and Thomas [2006], Exercise 8.6.
with respect to the generative natural parameters is:

\[ \frac{\partial B(\lambda)}{\partial \lambda} = \lambda \mathbb{E}_{p(z|x_\mu)}[\mathcal{M}(z)\mathcal{M}(z)] + \mathbb{E}_{p(z|x_\mu)}[\log p^{rec}(x_\mu|z)\mathcal{M}(z)]. \] \hspace{1cm} (3.9)

At optima or inflection points of \( B(\lambda) \), the derivative is zero and, if the moment matrix \( \mathbb{E}_{p(z|x_\mu)}[\mathcal{M}(z)\mathcal{M}(z)] \) is invertible, the generative natural parameters become:

\[ \lambda = -\mathbb{E}_{p(z|x_\mu)}[\log p^{rec}(x_\mu|z)\mathcal{M}(z)]. \]
\[ \mathbb{E}_{p(z|x_\mu)}[\mathcal{M}(z)\mathcal{M}(z)]^{-1}. \] \hspace{1cm} (3.10)

### 3.7 Gibbs machines.

It is clear from the above derivation that (3.7), (3.8) are universal for fully-generative nets and were hence used in the first fully-generative nets, the VAE-s [Kingma and Welling [2014], Rezende et al. [2014]. The VAE-s owe their name to the variational error term and were introduced in the context of very general sampling densities. Everything else being equal, the variational Pythagorean theorem (2.11) implies that latent sampling densities (2.13) from the Gibbs class minimize the generative error. Hence we call the respective nets Gibbs machines. While the variational error is due to an approximation, the variational principle from which the Gibbs class is derived, is fundamental to statistical mechanics.

### 3.8 Estimating variational error.

A closer look at the equilibrium identity for the natural parameters (3.10) reveals that it is identical to the maximum likelihood estimates of the coefficients of a linear regression:

\[ \log p^{rec}(x_\mu|z) = \alpha - \lambda \mathcal{M}(z) + \epsilon(x_\mu, z), \] \hspace{1cm} (3.11)

where \( \alpha \) is an intercept and \( \epsilon \) an error term. This observation was first made in [Richard and Zhang [2007] and later used in Salimans and Knowles [2013] to estimate variational error in the context of Variational Bayes. Adding \( \log p(z) \) to both sides, adding/subtracting \( F^{gen} \) to the right side, and recalling (2.13), (3.3), transforms (3.11) into:

\[ \log p(x_\mu, z) = \alpha - F^{gen} + \log p(z|x_\mu) + \epsilon(x_\mu, z). \] \hspace{1cm} (3.12)

Requiring \( \mathbb{E}_{p(z|x_\mu)}[\epsilon(x_\mu, z)] = 0 \) yields for the regression intercept the last expression in (3.8), with a negative sign:

\[ \log p(x_\mu, z) = -B(x_\mu) + \log p(z|x_\mu) + \epsilon(x_\mu, z). \] \hspace{1cm} (3.13)

The implied marginal density \( q(x_\mu) := \int p(x_\mu, z)dz \) is now:

\[ q(x_\mu) = e^{-B(x_\mu)}\mathbb{E}_{p(z|x_\mu)}[e^{\epsilon(x_\mu, z)}], \] \hspace{1cm} (3.14)

hence the cross-entropy for the \( \mu \)-th observation is:

\[ -\log q(x_\mu) = B(x_\mu) - \log \mathbb{E}_{p(z|x_\mu)}[e^{\epsilon(x_\mu, z)}], \] \hspace{1cm} (3.15)

i.e.

\[ D^{var}(x_\mu) = \log \mathbb{E}_{p(z|x_\mu)}[e^{\epsilon(x_\mu, z)}]. \] \hspace{1cm} (3.16)

This can be estimated either via Monte Carlo methods, or in a closed form. Assuming for example that \( \epsilon(x_\mu, z) \sim \mathcal{N}(0, \sigma(x_\mu)^2) \) is a Gaussian with variance \( \sigma(x_\mu)^2 \), yields

\[ D^{var}(x_\mu) = \sigma(x_\mu)^2. \]

While not rigorous, it is interesting to use these \( D^{var}(x_\mu) \) estimates, to train the neural net with the full cross-entropy \( -q(x_\mu) \) from (3.7), and not just its upper bound \( B(x_\mu) \) from (3.8) - see open problem 7, section 6.

### 3.9 Generative conditional independence.

Without offering a rigorous proof, we believe that the conditional independence argument from sub-section 2.2 can be generalized to this context: For a given reconstruction error, the generative error \( D^{gen} \) and hence the upper bound (3.8) is minimized when the latent variables are conditionally independent. For Gaussian multi-variate sampling, this follows from the explicit form of the generative error [Gil et al. [2013], table 3, and Hadamard’s inequality] [Cover and Thomas [2006], chapter 8.]

### 4 Latent symmetry statistics. Moments.

We will show for brevity only how to build spatial invariances in a 2-dim square visual recognition model. For real-life data sets, the symmetry statistics have to be computed via another net, see [Georgiev [2015b].]
Every observable i.e. pixel $x_i, i = 0, ..., N$, can be assigned a horizontal $h_i$ and a vertical $v_i$ integer coordinates on the screen, e.g., $h_i, v_i \in \{1, ..., \sqrt{N}\}$. In these coordinates, a row-observation $x_{\mu} = \{x_{\mu_{ii}}\}_{i=1}^{N}$ becomes a matrix-observation $\{ x_{\mu_{ii}}, v_i \}$ and a net layer of size $N$ becomes a layer of size $\sqrt{N} \times \sqrt{N}$. The center of mass $(h_{\mu}, v_{\mu})$:

$$h_{\mu} := \frac{\sum_{i=1}^{N} x_{\mu_{ii}} h_i}{\sum_i x_{\mu_{ii}}}, \quad v_{\mu} := \frac{\sum_{i=1}^{N} x_{\mu_{ii}} v_i}{\sum_i x_{\mu_{ii}}},$$

(4.1)

of every observation defines latent symmetry statistics $h = \{h_{\mu}\}_{\mu=1}^{P}$ and $v = \{v_{\mu}\}_{\mu=1}^{P}$, see sub-sections 1.6, 2.3.

Without loss of generality, we assumed here that $x_{\mu_{ii}} \geq 0$, hence $0 \leq h_{\mu}, v_{\mu} \leq \sqrt{N}$. In the coordinate system centered by $(h_{\mu}, v_{\mu})$, we have for every $\mu$ the new coordinates:

$$(\hat{h}_{\mu i}, \hat{v}_{\mu i}) := (h_i - h_{\mu}, v_i - v_{\mu}),$$

(4.2)

$-\sqrt{N} \leq \hat{h}_{\mu i}, \hat{v}_{\mu i} \leq \sqrt{N}$. In this coordinate system, every pixel has polar coordinates $r_{\mu i} := \sqrt{\hat{h}_{\mu i}^2 + \hat{v}_{\mu i}^2}, \varphi_{\mu i} := \text{atan2}(\hat{v}_{\mu i}, \hat{h}_{\mu i}) \in (-\pi, \pi]$, hence the new symmetry statistics: scale $r = \{r_{\mu}\}_{\mu=1}^{P}$ and angle $\varphi = \{\varphi_{\mu}\}_{\mu=1}^{P}$:

$$r_{\mu} := \frac{\sum_{i=1}^{N} x_{\mu} r_{\mu_{ii}}}{\sum_i x_{\mu_{ii}}}, \quad \varphi_{\mu} := \frac{\sum_{i=1}^{N} x_{\mu_{ii}} \varphi_{\mu i}}{\sum_i x_{\mu_{ii}}},$$

(4.3)

$0 < r_{\mu} \leq \sqrt{2N}, -\pi < \varphi_{\mu} \leq \pi$. In order to un-scale and un-rotate an image, change coordinates one more time to:

$$(\tilde{h}_{\mu i}, \tilde{v}_{\mu i}) := \frac{C}{r_{\mu}} (\hat{h}_{\mu i}, \hat{v}_{\mu i}) \left( \frac{\cos(-\varphi_{\mu})}{\sin(-\varphi_{\mu})} \frac{\sin(-\varphi_{\mu})}{\cos(-\varphi_{\mu})} \right),$$

(4.4)

$-M \leq \tilde{h}_{\mu i}, \tilde{v}_{\mu i} \leq M$, for some constants $C, M$ depending on $\min r_{\mu}, \max r_{\mu}$. After rounding and a shift, we thus have for any observation $\mu$, an index mapping:

$$\{1, ..., N\} \rightarrow \{1, ..., (2M + 1)^2\}$$

$$i \rightarrow \tilde{h}_{\mu i} + (\tilde{v}_{\mu i} - 1)(2M + 1).$$

(4.5)

When $2M + 1 > \sqrt{N}$, the $2M + 1 - \sqrt{N}$\,2 indexes which are not in the mapping image, correspond to identically zero observables for that observation. In the coordinates (4.4), a layer of size $N$ becomes a layer of size $(2M + 1)^2$.

In summary: i) for auto-encoders, apply mapping (4.5) at the input and its inverse at the output of the net; ii) for classifiers, apply mapping (4.5) at the input only; iii) for both, include in addition the symmetry statistics $h, v, r, \varphi$ in the latent layer, if needed, see Georgiev [2015b]. The prior model density $p()$ of symmetry statistics can be assumed equal to their parametrized posterior $p(\cdot|x_{\mu})$, but there are other options.

When sampling the symmetry statistics from independent Laplacians as in ([13]) e.g., the respective density means are set to be $h_{\mu}, v_{\mu}, r_{\mu}, \varphi_{\mu}$ from (4.1), (4.3). The density scales $\sigma_{h_{\mu}}, \sigma_{v_{\mu}}, \sigma_{r_{\mu}}, \sigma_{\varphi_{\mu}}$ on the other hand are free parameters, and can in principle be optimized in the non-creative regime, alongside the rest of the net parameters, sub-section 2.7. As argued in sub-section 1.6, the inverted scales are the scaled momenta. In the creative regime, when sampling e.g. from $\mathbf{h}$ alone, one will get horizontally shifted identical replicas. See open problem 2, section 6.

5 Experimental results.

The Theano Bastien et al. [2012] code used for experiments is in Georgiev [2015a], see also Popov [2015].

5.1 Non-generative ACE.

The motivation for the non-generative ACE comes from the Einstein observation entropies $\{-\log p^G(x_{\mu})\}_{\mu}$ as in sub-section 1.4, and their relation to singular value decomposition (SVD). Recall that the SVD of the $B \times N$ data matrix $\mathbf{X}$ with $B$ observations and $N$ observables is $\mathbf{X} = \mathbf{V} \mathbf{A} \mathbf{W}^T$. The $B \times B$ matrix $\mathbf{V} \mathbf{V}^T$ is i) a projection mapping; ii) its diagonals are up to a constant the negative Einstein observation entropies from sub-section 1.4, i.e., the Gaussian log-likelihoods $\{-\log p^G(x_{\mu})\}_{\mu}$; and iii) it is invariant on $\mathbf{X}$, i.e., $\mathbf{X} = \mathbf{V} \mathbf{V}^T \mathbf{X}$.

Let us consider a shallow auto-encoder, Figure 7, left, and its dual in the space of observations, Figure 7, right. It can be shown that for tied weights $\mathbf{V}^{(2)} = \mathbf{V}^{(1)^T}$, in the absence of non-linearities, the optimal $B \times N_{\text{hid}}$ hidden layer solution $\mathbf{H}_o$ on the left is $\mathbf{H}_o = \mathbf{V}^{(2)} = \mathbf{V}^{\text{Georgiev}}$.
1. Input layer:
   \( x_\mu \)
   Size = # observables \( N \)

2. Latent hidden layer:
   \( h_\mu = \phi(x_\mu W^{(1)} + b^{(1)}) \)
   Size = \( N_{lat} \)

3. Output layer:
   \( \hat{x}_\mu = \phi(h_\mu W^{(2)} + b^{(2)}) \)
   Size = \( N \)

---

1. Input layer:
   \( x_i \)
   Size = # observations \( P \)

2. Latent hidden layer:
   \( h'_i = \phi(V x_i + b^{(1)}) \)
   Size = \( N_{lat} \)

3. Output layer:
   \( \hat{x}_i = \phi(V^{(2)} h'_i + b^{(2)}) \)
   Size = \( P \)

---

Figure 7: Shallow auto-encoder in the space of observables (left) and observations (right). Minimization targets are the reconstruction errors in the respective spaces \(- \log \mathcal{L}_{\text{recon}}\) and \(- \log \mathcal{L}'_{\text{recon}}\) defined for binarized data in Appendix A, \( \phi, \varphi \) are non-linearities.

[2015c]. The divergence of \( V V^T X \) from \( X \) is thus the reconstruction error in the dual space and minimizing it gets us closer to the optimal \( H_0 \). If we treat the first hidden layer \( H \) of a classifier as the rescaled dual weight matrix \( \sqrt{B} V^{(2)} \), we arrive at the dual reconstruction error:

\[
- \log \mathcal{L}'_{\text{recon}} = \frac{1}{B} \sum_{i=1}^{N} \mathbb{E}_{x_i} [- \log \varphi(HH^T x_i / B)],
\]

(5.1)

for a given column-vector observable \( x_i = \{ x_{\mu i} \}_{\mu=1}^{B} \) and sigmoid non-linearity \( \varphi() \), see Appendix A.

The non-generative ACE has as minimization target the composite cross-entropy (1.4), with \(- \log \mathcal{L}_{AE} \) replaced by the dual reconstruction error (5.1). The orthogonality \( V^T V = I_{N_{lat}} \) of \( V \) implies the need for an additional batch normalization, similar to Ioffe and Szegedy [2015], see Appendix A.

The best known results for the test classification error of feed-forward, non-convolutional nets, without artificial data augmentation, are in the 0.9-1% handle Srivastava et al. [2014], table 2. As shown on the right of Figure 8, the non-generative ACE offers a 20-30% improvement.

5.2 Generative ACE.

The architecture is in Figure 5, the minimization target is the ACE cross-entropy (1.4), with \(- \log \mathcal{L}_{AE} \) replaced by the upper bound (3.8). Laplacian sampling density is used in training and the mixed Laplacian in testing, with the explicit formulas for the generative error in Appendix B. The generative ACE produces similarly outstanding clas-
sification results as the non-generative ACE on the regular MNIST data set, Figure 9 left. Even without tweaking hyper-parameters, it also produces outstanding results for the density estimation of the binarized MNIST data set, Figure 9 right. An upper bound for the negative log-likelihood in the 86-87 handle is in the ballpark of the best non-recurrent nets, [Gregor et al. 2015], table 2.

Figure 9: Left. Classification error for the MNIST 10000 test set. Top line is from a standard classifier net as on the right of Figure 1. Bottom lines are from generative ACE in classification mode: Gaussian sampling (red) and Laplacian (green). Layer sizes 784-700-(100x10)-(700x10)-(784x10) for the AE branch and 784-700-700-700-10 for the C branch, Figure 5 and Appendix A, learning rate = 0.0015, decay = 500 epochs, batch size = 10000. The dual reconstruction error \( -\log L_{recon} \) from sub-section 5.1 is added to the overall cost. Right. Upper bound (3.8) of the negative log-likelihood for the binarized MNIST 10000 test set. The top line is the standard Gibbs machine with Gaussian sampling, layer sizes 784-700-400-700-784 and other hyper-parameters as below. The middle line is the same net but with Laplacian sampling. The bottom line is generative ACE with Laplacian mixture sampling. Layer sizes 784-700-(400x10)-(700x10)-(784x10) for the AE branch and 784-700-700-700-10 for the C branch, Figure 5 and Appendix A, learning rate = 0.0002, decay = 500 epochs, batch size = 1000.

6 Open problems.

1. Use the freely available intricates, sub-section 1.5 directly as feature detectors, in lieu of artificially computed Independent Component Analysis (ICA) features [Hyvarinen et al. 2009].
2. Test empirically the performance of ACE, with the symmetry statistics added as in section 4, computed either in closed form, or from specialized nets, as in [Jadeberg et al. 2015]. For the distorted MNIST and CIFAR10 datasets, see [Georgiev 2015].
3. Deepen and make generative the shallow dual encoder of the non-generative ACE, sub-sections 1.7 and 5.1 here.
4. Test empirically q-Gibbs machines, with cross-entropies replaced by their q-equivalents and sampling from q-Gibbs densities, sub-section 2.10 here.
5. Improve the upper bound for the generative error of mixture densities in Appendix B by using variational methods as in [Hershey and Olsen 2007].
6. How is the ACE blend of exponential and mixture densities related to the beautiful duality between these two families, underlying information geometry [Amari and Nagaoka 2001], section 3.7?
7. Estimate the variational error (3.4) [Richard and Zhang 2007, Salimans and Knowles 2013] and use it in training to minimize the full cross-entropy, not merely its upper bound, as suggested in sub-section 3.8 here.

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Appendices

A Software and implementation.

The optimizer used is Adam [Kingma and Ba 2015] stochastic gradient descent back-propagation. Specific hyper-parameters are in the text. We used only two standard sets of hyper-parameters, one for the classifier branch and one for the auto-encoder branch, no optimizations.

For reconstruction error of a binarized $\mu$-th row-observation $x_\mu = \{x_{\mu i}\}_{i=1}^N$ and its reconstruction $\hat{x}_\mu$, we use the standard binary cross-entropy Bastien et al. [2012]:

$$E_{x_\mu}[-\log \hat{x}_\mu] = \sum_i (-x_{\mu i} \log \hat{x}_{\mu i} - (1 - x_{\mu i})(1 - \log \hat{x}_{\mu i})),$$

using a sigmoid last non-linearity $\varphi$. The batch cross-entropy is $-\log L_{\text{recon}} = \frac{1}{B} \sum_{\mu=1}^B E_{x_\mu}[-\log \hat{x}_\mu]$. In the space of observations, as on right plot of Figure 7 the dual reconstruction error is the same binary cross-entropy $E_{x_i}[-\log \hat{x}_i]$, but for the $i$-th observable $x_i = \{x_{\mu i}\}_{\mu=1}^P$ and a sum over $\mu$ instead of $i$. The batch cross-entropy is $-\log L'_{\text{recon}} = \frac{1}{B} \sum_{i=1}^N E_{x_i}[-\log \hat{x}_i]$, with a normalization factor conforming to the space of observables.

The non-linearities are $\tanh()$ in the auto-encoder branch and two-unit maxout Goodfellow et al. [2013] in the classifier branch. Weight matrices of size $P \times N$ are initialized as random Gaussian matrices, normalized by the order of magnitude $\sqrt{P} + \sqrt{N}$ of their largest eigenvalue. As discussed in sub-section 5.1 hidden observables in the first and last hidden layer of classifiers are batch-normalized i.e. de-meaned and divided by their second moment. Unlike Ioffe and Szegedy [2015], batch normalization is enforced identically in both the train and test set, hence test results depend slightly on the test batch.

B Generative error formulas.

When sampling from a Laplacian, in order to have an unity variance in the prior, we choose for the independent one-dimensional latents a prior $p(z) = p^{\text{Lap}}(z; 0, \sqrt{0.5})$, where $p^{\text{Lap}}(z; \mu, b) = \exp(-|z - \mu|/b) / (2b)$ is the standard Laplacian density with mean $\mu$ and scale $b$. In order to have zero generative error when $(\mu, \sigma) \to (0, 1)$, we parametrize the conditional posterior as $p(z|.) = p^{\text{Lap}}(z; \mu, \sigma\sqrt{0.5})$. The generative error in (3.8) equals:

$$- \log \sigma + |\mu|/\sqrt{0.5} + \sigma \exp(-|\mu|/(\sigma\sqrt{0.5})) - 1,$$

see Gil et al. [2013], table 3.

For the divergence between a mixture prior $\sum_s \alpha_s p_s(z)$ and a mixture posterior $\sum_s \alpha_s p_s(z|.)$ with the same weights $\{\alpha_s\}_s$, we use the upper bound $\sum_s \alpha_s D(p_s(z|.) || p_s(z))$ implied by the log sum inequality (Cover and Thomas 2006). For improvements, see open problem 5 in section 6.