Saddlepoints in Unsupervised Least Squares

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Abstract

This paper sheds light on the risk landscape of unsupervised least squares in the context of deep auto-encoding neural nets. We formally establish an equivalence between unsupervised least squares and principal manifolds. This link provides insight into the risk landscape of auto-encoding under the mean squared error, in particular all non-trivial critical points are saddlepoints. Finding saddlepoints is in itself difficult, overcomplete auto-encoding poses the additional challenge that the saddlepoints are degenerate. Within this context we discuss regularization of auto-encoders, in particular bottleneck, denoising and contraction auto-encoding and propose a new optimization strategy that can be framed as particular form of contractive regularization.

1 Introduction

This paper examines the risk landscape of unsupervised least squares. Unsupervised least squares aims to find a reconstruction map \( r \) that minimizes the discrepancy of the output to its own input, i.e., minimizing \( \| r(x) - x \|^2 \). In the neural network literature this is referred to as auto-encoding. Without any restrictions on \( r \) the identity mapping is an optimal, albeit uninformative, solution. An informative solution should provide a salient summary of the data. To find informative solutions, auto-encoding is typically formulated as a concatenation of an encoder map \( \lambda \) and a decoder map \( g \) with \( r = g \circ \lambda \) with restrictions on \( \lambda \) or \( g \) to avoid learning the identity function. Several regularization methods exist to enforce such restrictions. For example, the bottleneck auto-encoder forces the map \( \lambda \) to be of lower dimension than the input through adding a bottleneck layer. While such regularization avoid learning the identity map, they do not address the general problem of overfitting in unsupervised least squares.

For networks with linear activations, [Kawaguchi, 2016] show that for auto-encoding all minima are globally optimal and the solutions correspond to the maximal principal subspace. This paper provides an analogous characterization of the critical points of the risk function for deep auto-encoders in the non-linear case. In particular all critical points, besides minima with zero risk, are saddle points. Zero risk solutions defy the purpose of autoencoders, i.e. finding a more compact representation that characterizes the input data. In the linear case solution with zero risk are identity functions. Zero In the non-linear case zero risk solutions include, besides the identity, space filling manifolds. This highlights an important distinction between the linear and non-linear case. In the linear case it is
sufficient to restrict the dimensionality of the principal subspace, for example through the use of a bottleneck layer. For non-linear auto-encoders additional regularization of the encoding and decoding functions is required, otherwise the optimization will tend towards space-filling solutions.

We establish a tight connection between unsupervised least squares and the more restrictive notion of a principal manifold. This connection illuminates the risk landscape of unsupervised least squares, which in turn informs the behaviour of auto-encoding under various forms of regularization. Hastie and Stuetzle [1989] formally defined principal curves as curves that pass through the middle of a distribution and showed that principal curves are critical points of the mean squared reconstruction error. This indicates a tight connection to unsupervised least squares. Principal manifolds enforce that the reconstruction function constitutes an orthogonal projection, while unsupervised least squares permit arbitrary reconstruction functions. To establish the equivalence between principal manifolds and unsupervised least squares we show that the critical points of the mean squared error risk for arbitrary reconstruction functions, and thus the critical points of auto-encoders under squared error loss, are principal manifolds. The connection of unsupervised least squares to principal manifolds illuminates the shape of the auto-encoder risk landscape. In particular Duchamp and Stuetzle [1996] showed that principal curves are saddlepoints of the mean squared error, this observation also holds for auto-encoding. Duchamp and Stuetzle [1996] and Gerber and Whitaker [2013] demonstrate that the saddlepoint nature of the risk landscape leads to overfitting and renders traditional cross-validation techniques infeasible for tuning of regularization parameters.

This difficulty persists for auto-encoders as Figure 1 illustrates in the case of bottleneck auto-encoding. The bottleneck layer enforces a hard constraint on the dimensionality of the reconstruction function, while the network architecture implicitly regularizes the complexity of the reconstruction function. However, due to the saddlepoint nature of the risk landscape the risk on test data keeps decreasing with increasing network complexity. Thus, cross-validation will fail to suggest an appropriate network complexity. In the limit, with infinite training data and no restriction on the complexity of the reconstruction function a space filling curve, with zero reconstruction error, is an optimal fit. These global minima, space-filling manifolds or the identity function, of the auto-encoding risk are not desirable solutions and do not provide an adequate summary representation of the data. The hard dimensionality constraint in bottleneck auto-encoders avoids fitting the identity function. However, the hard constraint requires careful initialization to find an adequate parametrization. As an alternative to the bottleneck layer several regularization schemes, such as denoising [Vincent et al., 2008] and contractive auto-encoding [Alain and Bengio, 2014], for controlling the dimensionality of the reconstruction function have been proposed. These regularization methods provide a soft constraints on dimensionality and solve or circumvent the issue of tuning preparametrization. The soft dimensionality constraints do not alleviate the challenge of tuning the regularization or selecting an appropriate network architecture. Figure 2 shows that for a fixed contractive penalty the test error for different network architecture either selects an architecture that severely overfits or tends towards the identity mapping. Fixing the network architecture while adjusting the regularization does not solve the issue as Figure 3 illustrates. A very flexible network that permits severe overfitting leads to the smallest test error. If the network architecture is restrictive enough
Figure 1: Bottleneck auto-encoding enforces a hard dimensionality constrain through a bottleneck neural network layer. The images show (top row) the minima found after 20,000 iterations and (bottom row) the root mean square error on training (green solid line) and test data (purple dashed line) using network architectures with hidden layers of (a) 50–100–200–100–50–1–50–100–200–100–50, (b) 50–100–50–1–50–100–50, (c) 200–1–200 units. Depending on the network architecture, auto-encoding does (a) overfit, (b) fit well or (c) underfit. The relatively small reach of the spiral example requires a fairly deep network to achieve an accurate fit. However, the test error does not suggest that the fit in (b) is adequate and suggests to use the most powerful network. In all cases the one-dimensional parametrization of the auto-encoder jumps across the spiral arms.

the test error decreases with decreasing penalty weight and the solution tends towards the identity mapping. In practice the structure in the data is typically not know and it would be difficult to select an appropriate network architecture. Thus, a method that imposes a dimensionality constraint without reliance on the implicit regularization of the network architecture is desirable. We contend that the difficulties in regularization of auto-encoders are due to the saddlepoint structure of the unsupervised least squares risk.

The critical points of the unsupervised least squares risk are principal manifolds and provide an arguably reasonable summary representation of the data. However, except for the uninformative identity solution and space filling manifolds the critical points are saddlepoints. Figures Figures[1][2] and [3] illustrate that the saddlepoint nature of the critical points renders cross-validation useless, since it is possible to move away from a critical point without increasing the risk on test data. Furthermore steepest decent methods will typically not even move towards desirable solutions. In the principal manifold setting, Gerber and Whitaker [2013] propose a solution to the saddlepoint challenge based on minimizing a different risk. The novel risk has the property that principal manifolds are now minima instead of saddlepoints. We show that this risk, derived from geometrical considerations,
Figure 2: Effect of network architecture in combination with contractive regularization penalty. The image show the (top row) minima found after 20,000 iterations and (bottom row) the root mean square error on training (green solid line) and test data (purple dashed line) using a fixed penalty of 0.02 and network architectures with hidden layers of (a) 50–100–200–200–100–50, (b) 50–100–100–50, (c) 200–200 units. The gray lines show a polar grid on the input space and the black lines show the deformation of the polar grid after mapping it through the auto–encoder. The gray line shows the spiral the data is sample from with noise. The black lines shows the spiral after mapping it through the auto–encoder.

is a particular application of a more general approach based on minimizing the norm of the Gradient of the risk. We apply this Gradient–Norm minimization to auto–encoders, which results in a formulation that bears a close resemblance to contractive auto–encoding \cite{Alain and Bengio, 2014}.

2 \ The Unsupervised Least Squares Risk

This section shows that the critical points of the unsupervised least squares risk are principal manifolds and investigates the properties of those critical points in detail. Section 2.1 revisits the definition of a principal curves and manifolds and Section 2.2 establishes the connection of the unsupervised least squares risk to principal manifolds by examination of the first variation of the unsupervised least squares risk.

2.1 Connection to Principal Manifolds

Let X be a random variable with a smooth density $p$ such that the support $\Omega = \{x : p(x) > 0\}$ is a compact, connected region with smooth boundary. Denote by $E$ the expectation operator, i.e., $E[f(X)] = \int_{\Omega} f(x)p(x)dx$.

Recall the formal definition of principal curves.

**Definition 2.1** (Principal Curve \cite{Hastie and Stuetzle, 1989}). Let $g : \Lambda \to \mathbb{R}^n$, $\Lambda \subset \mathbb{R}$ and
Figure 3: Effect of regularization penalty for fixed network architecture. The image show
the (top row) minima found after 20,000 iterations and (bottom row) the root mean square
error on training (green solid line) and test data (purple dashed line) using a network ar-
chitecture with hidden layers of 50–50–50–50 units and regularization weights (a) 0.04 (b)
0.02 and (c) 0.005. The gray lines show a polar grid on the input space and the black lines
show the deformation of the polar grid after mapping it through the auto–encoder.

\( \lambda_f : \Omega \to \Lambda \) with projection index \( \lambda_f(x) = \max \{ s : \| y - g(x) \| = \inf \| y - g(\tilde{x}) \| \} \). The
principal curves of \( Y \) are the set \( \mathcal{G} \) of smooth functions \( g \) that fulfill the self consistency
property \( E[Y|\lambda_f(X) = z] = g(z) \).

[Hastie and Stuetzle (1989)] showed that principal curves are critical points of the risk
\( d(g, X)^2 = \frac{1}{2} E[\| g(\lambda_f(X)) - X \|^2] \). The principal curve risk is closely related to the unsupervised
learning risk, but imposes restriction on the form of the decoder \( \lambda \), i.e., the encoder
\( \lambda \) is forced to be the projection index given \( g \).

The typical approach to estimate principal curves optimizes over \( g \) and solver the non–linear problem of finding \( \lambda_f \). To circumvent the non–linear optimization problem of computing \( \lambda_f \), [Gerber et al. 2009] proposed a new formulation that switches the optimization
over the encoder \( \lambda \) while fixing \( g(\lambda_f(z)) \approx E[X|\lambda_f(X) = z] \) to be the conditional expectation
given \( \lambda \). This yields the risk \( d(\lambda, X)^2 = \frac{1}{2} E \left[ \| g(\lambda_f(X)) - X \|^2 \right] \). Again closely related to
the unsupervised least squares risk but with restrictions imposed on the form of the decoder
\( g \).

For future reference we term the three different formulations as:
1. Principal manifold risk (pm–risk): \( d(g, X)^2 \) with \( \lambda_f \) constrained to be orthogonal to
\( g \).
2. Conditional expectation manifold risk (cem–risk): \( d(\lambda, X)^2 \) with \( g \) constrained to the conditional expectation given \( \lambda \).
3. Unsupervised least squares risk (uls–risk): \( d(g, \lambda, X)^2 \) with \( g \) and \( \lambda \) unconstrained.[Duchamp and Stuetzle (1996)] showed that principal curves are saddlepoints of the pm–risk
\( d(g, X)^2 \) and [Gerber and Whitaker (2013)] showed that critical points of the cem–risk are
weak principal curves. Weak principal curves are, as the name implies, a slightly weaker version of principal curves:

**Definition 2.2** (Weak Principal Curves [Gerber and Whitaker, 2013]). Let $g : \Lambda \to \mathbb{R}^n$ and $\lambda : \Omega \to \Lambda$. The weak principal curves of $Y$ are the set $G_w$ of functions $g$ that fulfill the self consistency property $E[Y|\lambda(Y) = s] = g(s)$ with $\lambda$ satisfying $\langle y - g(\lambda(y)), \frac{dg(s)}{ds} \big|_{s=\lambda(y)} \rangle = 0 \forall y \in \Omega$.

For principal curves which have no ambiguity points, i.e. all $x \in \Omega$ have a unique closest point on the curve, the definition is equivalent to principal curves.

### 2.2 Critical Points are Principal Manifolds

To establish the connection of the unsupervised least squares risk $d(g, \lambda, X)^2 = \frac{1}{2} E \left[ \|g(\lambda(X)) - X\|^2 \right]$ to principal manifolds, we show that the critical points of $d(g, \lambda, X)^2$ are weak principal manifolds.

For the pm–risk the optimization is over decoder $g$ only the encoder $\lambda$ is defined in terms of $g$. Vice versa, for the cem–risk the optimization is over the encoder $\lambda$ only and the decoder $g$ is defined in terms of $\lambda$. The following theorem establishes that the critical points for the uls–risk which includes optimization over both $g$ and $\lambda$ are weak principal manifolds.

**Theorem 2.1.** The critical points of the unsupervised least squares risk $d(g, \lambda, X)^2 = \frac{1}{2} E \left[ \|g(\lambda(X)) - X\|^2 \right]$ are weak principal curves.

**Proof.** The Gâteaux derivative (or first variation) of $d(\lambda, g, X)^2$ with respect to $\lambda$ is

$$d(\lambda + \varepsilon \tau, g, X)^2 = E \left[ (g(\lambda(X) - X)) \nabla g(\lambda(X)) \tau(X) \right]$$ (1)

and with respect to $g$

$$d\varepsilon d(\lambda, g + \varepsilon h, X)^2 = E \left[ (g(\lambda(X)) - X, h(\lambda(X))) \right].$$ (2)

At a critical point these have to be pointwise zero for any $\tau$ (variation of $\lambda$) and $h$ (variation of $g$), respectively. This yields the conditions $\langle g(\lambda(X) - X) \nabla g(\lambda(X)) \rangle = 0$ from equation (1) and $g(z) = E[X \{ x : \lambda(x) = z \}]$ for any $z$ in the image of $\lambda$ from equation (2). This establishes that critical points of the uls–risk are weak principal manifolds.

The critical points contain uninteresting minimal solutions with zero reconstruction residual, i.e., space filling manifolds and the identity mapping. Critical points of the pm–risk and cem–risk are saddlepoints, since the uls–risk is more flexible, i.e., is a superset of both the pm–risk and the cem-risk, the critical points of the uls–risk are saddlepoints as well.
The uls–risk poses additional challenges. If \( \lambda \) is permitted to be injective, i.e., no dimensionality constraints, then the condition that \( g(z) = E[X|\{x: \lambda(x) = z\}] \) can only be satisfied by the identity mapping, since the set \( \{x: \lambda(x) = z\} \) is a single point. Additionally, in that setting the critical points have a discontinuous Gâteaux derivative: Consider a critical point with encoder \( \lambda^* \) and decoder \( g^* \), with rank \( \nabla \lambda \) less than \( n \). Let \( \pi_\alpha \) be a set of maps such that \( \lambda + \pi_\alpha \) is injective and \( \|\pi_\alpha(x)\| \leq \alpha \). Now from the critical point conditions \( \int_{\lambda^{-1}(\{z\})} (g(z) - x) p(x) dx = 0. \) Let \( s = (\lambda + \pi_\alpha)^{-1}(\{z\}) \), now for any \( \alpha > 0 \) we have \( \int_{(\lambda + \pi_\alpha)^{-1}(\{z\})} (g(z) - x) p(x) dx = (g(s) - x) p(x) + \alpha \|\nabla g(s)\| + O(\alpha^2) \) which cannot be made arbitrarily small. This discontinuity is expected since the expectation \( E \) changes abruptly when moving to an injective function, or in fact at any change in the rank of the Jacobian \( \nabla \lambda \). Thus, in order to avoid the identity mapping it is necessary to constrain the dimensionality of the reconstruction function.

3 Shaping the Unsupervised Least Squares Risk

To avoid fitting overly curved solutions [Rifai et al. 2011] propose an explicit penalty on the shape of the solution by adding a penalty on the Hessian to contractive encoding. This approach combines a regularization on the dimensionality, the Jacobian, and a regularization on the curvature, the Hessian. Penalizing the Hessian is akin to the proposal by [Kégl et al. 2000] in the context of fitting principal manifolds. However, the saddlepoint nature of the objective function makes it infeasible to use cross-validation for tuning the amount of regularization required.

To address the saddlepoint challenge we propose to change the objective function such that all critical points are local minima. Gerber and Whitaker [2013] applied this approach to principal manifolds. They observed that principal curves are saddlepoints of the risk because curves with smaller risk can be achieved by either violating the conditional expectation constraint in the pm–risk or by violating the orthogonality constraint in the cem–risk formulation. This lead Gerber and Whitaker [2013] to minimize orthogonality using the risk:

\[
q(\lambda, X)^2 = E \left[ \left( \frac{d}{dz} g(\lambda(X)) - X \right)^2 \right] = 0. \tag{3}
\]

Gerber and Whitaker [2013] showed that all critical points of this risk are minima and principal curves.

In this section we show that there is a general principle underlying the derivation by Gerber and Whitaker [2013] that is not restricted to the principal manifold case. In Section 3.1 we derive the general principle from Newton’s method for optimization and show how it leads to the orthogonal risk in the case of principal manifolds and in Section 3.3 we apply it to auto–encoding which results in an orthogonal contractive penalty.

3.1 Gradient–Norm Minimization

Newton’s method for finding critical points of a function \( f : \mathbb{R}^m \to \mathbb{R} \) is to find the zero crossings of \( \nabla f \). Newton’s method applied to the gradient of a multivariate function \( f : \mathbb{R}^m \to \mathbb{R} \) :
\( \mathbb{R}^m \to \mathbb{R} \) yields updates of the form

\[ x^{k+1} = x^k - \alpha v \]

with \( v \) a solution to

\[ \nabla^2 f(x^k) v = \nabla f(x^k) \]

where \( \nabla^2 f \) is the Hessian of \( f \). For \( \nabla^2 f \) indefinite the iterations moves—given an appropriate step size—towards a saddlepoint.

If the Newton step is difficult to solve, i.e., the inversion of the Hessian to expensive, one can resort to minimizing the gradient norm \( ||\nabla f(x)||^2 \). Since \( ||\nabla f(x)||^2 \geq 0 \), the critical points of \( f \) are minima of the gradient–norm risk. However, depending on the structure of \( f \), additional critical points are possible. At critical points of \( ||\nabla f(x)||^2 \) the gradient \( \nabla^2 f(x) \nabla f(x) \) has to be zero. Thus, either the gradient \( \nabla f \) has to be zero, the Hessian \( \nabla^2 f \) is zero or the gradient is a linear combination of directions with zero curvature, i.e. \( \nabla f v = 0 \) or \( \nabla^2 f v = 0 \) for all directions \( v \). For functions with non-degenerate Hessians, inflection points in the direction of the gradient are additional critical points of \( ||\nabla f||^2 \). Such critical points can pose a problem for finding critical points of \( f \) through gradient–norm minimization and need to be evaluated.

Newton’s method is a scaled steepest descent method with scaling by \( \nabla^2 f(x)^{-1} \). The gradient of \( \nabla f(x) \) is \( \nabla^2 f(x) \nabla f(x) \), i.e., a steepest descent with scaling by \( \nabla^2 f(x) \). This avoids having to invert the Hessian but worsen the condition number and results in slower convergence [Boyd and Vandenberghe 2004].

### 3.2 Gradient–Norm Minimization for Principal Manifolds

Applying the gradient-norm minimization procedure to the cem–risk recovers the geometrically derived formulation by [Gerber and Whitaker 2013]. The gradient of \( d(\lambda, X)^2 \) with respect to \( \lambda \) is:

\[ E \left[ \left( g_\lambda(\lambda(X)) - X, \frac{d}{ds} g(s) \bigg|_{s=\lambda(X)} \right) \right]. \quad (4) \]

By the calculus of variations this has to hold pointwise. Applying the gradient–norm minimization pointwise recovers the orthogonality risk in Equation[3]

### 3.3 Gradient–Norm Minimization for Auto–encoding

Applying the gradient-norm minimization to the uls–risk from Equations [1] and [2] results in the risk:

\[ E \left[ (g(\lambda(X)) - X)^2 \right] + \alpha E \left[ (g(\lambda(X)) - X)^2 \nabla g(\lambda(X))^2 \right] \]

with \( \alpha = 1 \). The first term is the squared residual and the second term can be seen as a directional contraction penalty; the Jacobian of \( g \) is penalized but only in the direction of the residual vector. For principal manifolds the second term is zero since the Jacobian of \( g \) has to be zero in the direction of the residual, i.e. \( g \cdot \lambda \) is an orthogonal projection to \( g \).
Treating the second term of the derivative as a penalty we can weigh it differently through changing $\alpha$ during optimization.

Figure 4 illustrates this approach on a bottleneck neural network architecture and compares it with no and contractive regularization.

Figure 4: The image show the minima found after 20,000 iterations using a network architecture with hidden layers of 50–100–200–1–200–100–50, units and (a) no regularization (b) contraction penalty and (c) orthogonal contractive penalty.

Figure 5: The effect of the orthogonal contractive penalty on an idealized example problem. The idealized setting assumes that the Jacobian norm is perfectly anti–correlated with the residual. That is, as the reconstruction functions moves away from the identity function (at $x - r(x) = 0$) towards a principal manifold (at $x - r(x) = 1$) the increase in error is matched by a decrease in the Jacobian. The orthogonal contraction has a minima at both 0 and 1, but combined with the squared residual term, the effect is negligible. Increasing the orthogonal penalty creates a minima closer to the principal manifold, however, the identity function still is minimal and has a larger region of attraction. The normalized orthogonal penalty actively pushes the solution away from the identity solution and combined with the residual term leads to a minima close to the principal manifold.

The method for finding saddlepoints does not address the issue of discontinuous saddlepoints if the dimensionality is not restricted. The orthogonal contractive penalty does typically not help to find such degenerate solutions and results in the identity solution. This behaviour is expected since moving towards the identity solution often also reduces the orthogonal contractive penalty as illustrated in an idealized setting in Figure 5. To remedy
this problem we consider normalizing the contractive penalty to:

\[ \alpha E \left[ \frac{(g(\lambda(X)) - X)^2 \nabla g(\lambda(X))^2}{(g(\lambda(X)) - X)^2} \right]. \]  

(6)

This has the effect that the penalty increases quadratically towards the identity solutions, as illustrated in Figure 5. The normalized penalty counterweights the quadratic decrease in the reconstruction error. Figure 6 demonstrates the desired effect of pushing the solution away from the identity.

Figure 6: The image show the minima found after 20,000 iterations using a network architecture with hidden layers of 50–100–200–100–50, units and (a) 0.04 (b) 0.02 (c) 0.005 weighted orthogonal penalty. The orthogonal penalty yields reasonable results for a range of penalty weights.

The orthogonal penalty works well for examples with a co-dimension of one. For more realistic examples, with higher co-dimension, the orthogonal penalty reaches zero if the residual vectors are contained in any subspace of the normal bundle. In this case the orthogonal contractive penalty has to be combined with a dimensionality constraint. Figure 7 shows the effect on denoising auto-encoding. The orthogonal contractive penalty preferentially selects directions that tend towards an orthogonal projection.

Figure 7: The (a) illustration depicts the effect of orthogonal contraction with denoising auto-encoding. In the limit, points from the density (gray area) with noise added, \( x + \varepsilon \) (black dot) are preferentially mapped orthogonal to the contraction (purple) as compared to denoising alone (orange). The (b) orthogonal contraction with denoising leads to sharper boundary as compared to (c) denoising alone. This indicates that orthogonal contraction with denoising can yield solutions that generalize better to unseen data than denoising alone.
4 Conclusion

The connection of auto-encoding neural networks with principal manifolds casts regularization as an approach to find saddlepoints of the mean squared error risk. The issue of saddlepoints has been recently explored in the neural network literature. Pascanu et al. [2014] develop an optimization strategy to avoid saddlepoints, while Choromanska et al. [2015] argue that saddlepoints are desirable solutions in deep learning. The connection to principal manifolds makes the argument for saddlepoints as desirable solutions explicit in the case of auto-encoding networks.

We proposed a new method, gradient-norm minimization for finding saddlepoints. The gradient-norm minimization is potentially converging slowly. Both Newton’s method and gradient-norm minimization are gradient descent schemes under scaling. Newton’s method scales by the inverse Hessian, while the proposed method corresponds to a scaling by the Hessian. This scaling increases the condition number and decreases the convergence rate.

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