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Topology of the loss landscape: global and local structures

Theories of Deep Learning: C6.5,
Lecture / Video 9

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Consider a data set $X \in \mathbb{R}^{n \times m}$ of m data entries in $\mathbb{R}^n$, associated target outputs (such as labels) $Y \in \mathbb{R}^{n_2 \times m}$ (for simplicity we let $n_2 = n$), and (very) simple two layer net:

$$\begin{aligned} h_1 &= \phi(W^{(1)} x_0) \quad \text{note, no bias, and } \phi(\cdot) = \max(0, \cdot) \\ h_2 &= W^{(2)} h_1 \quad \text{note, no bias or nonlinear activation.} \end{aligned}$$

The output of the net is $H(x_\mu; \theta) = \hat{y}_\mu$ and we measure the value of the net through the average sum of squares:

$$\mathcal{L} = (2m)^{-1} \sum_{\mu=1}^{m} \sum_{i=1}^{n} (\hat{y}_{i,\mu} - y_{i,\mu})^2$$

and define a weighted loss accuracy as $\epsilon = n^{-1}\mathcal{L}$.

Loss landscape example: 56 layers fully connected (Li et al. 18')

Loss landscapes of DNNs are typically non-convex

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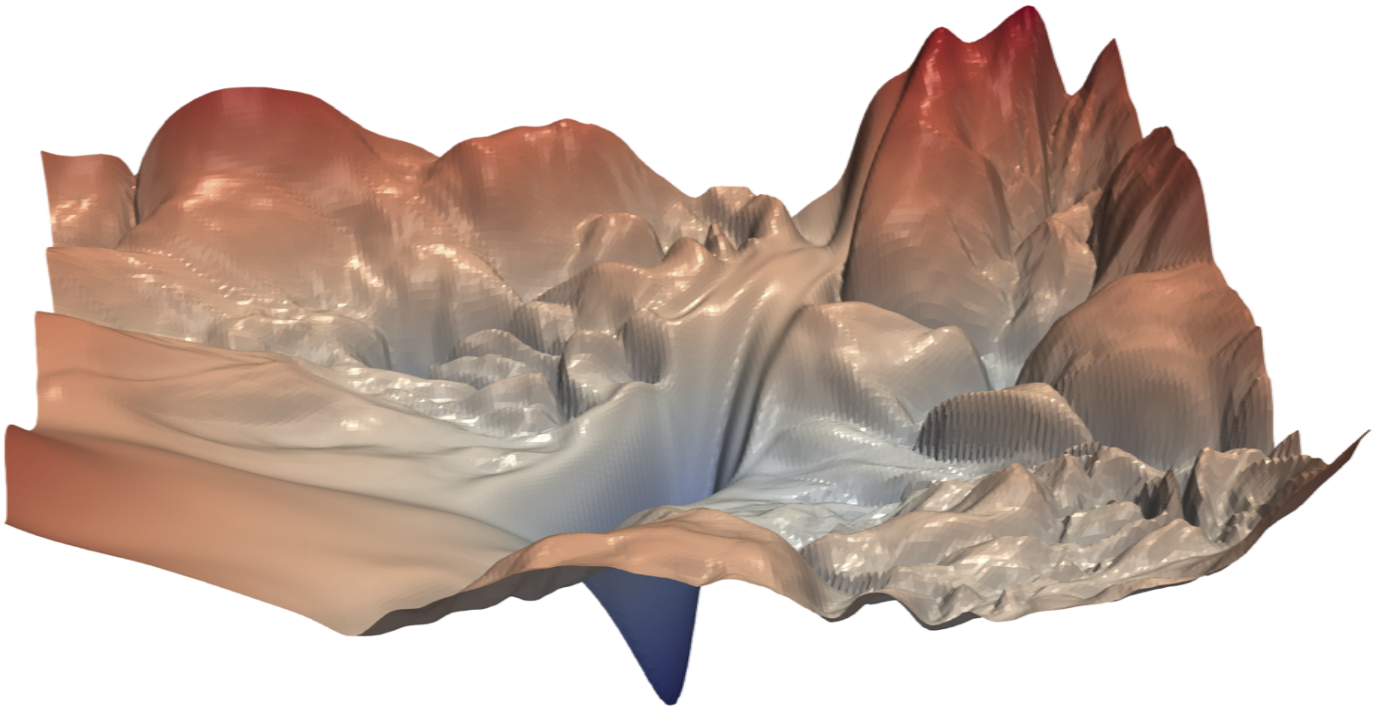

http://papers.nips.cc/paper/7875-visualizing-the-loss-landscape-of-neural-nets.pdf

Topology of loss landscape (Freeman et al. 16')

Number of connected components

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Consider our loss function: $\mathcal{L}(\theta; X, Y) = n^{-1} \sum_{\mu=1}^{n} l(\theta; x_\mu, y_\mu)$ and its associated level set

$$\Omega_{\mathcal{L}}(\lambda) = \{\theta : \ \mathcal{L}(\theta; X, Y) \leq \lambda\}$$

Of particular interest are the number of connected components, say N_λ, in $\Omega_{\mathcal{L}}(\lambda)$. If $N_\lambda = 1$ for all λ then $\mathcal{L}(\theta; X, Y)$ has no isolated local minima and any descent method can obtain a global minima.

If $N_\lambda > 1$ there may be "spurious valleys" in which the minima in the connected component does not achieve the global minima. `https://arxiv.org/pdf/1611.01540.pdf`

Topology of loss landscape (Freeman et al. 16')

There are datasets for which ReLU has a complex landscape

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Linear network: single component

Let $H(x;\theta)$ be an L layer net given by $h^{(\ell)} = W^{(\ell)} h^{(\ell-1)}$ with $W^{(\ell)} \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$, then if $n_\ell > \min(n_0, n_L)$ for $0 < \ell < L$, the sum of squares loss function has a single connected component

ReLU network: multiple components

Let $H(x;\theta)$ be an L layer net given by $h^{(\ell)} = \sigma(W^{(\ell)} h^{(\ell-1)})$ with $W^{(\ell)} \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$ and $\sigma(\cdot) = \max(0, \cdot)$, then for any choice of n_ℓ there is a distribution of data (X, Y) such that there are more than one single connected component.

Topology of loss landscape: (Venturi et al. 16')

Over parameterisation can generate a single connected component

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ReLu activation network: nearly connected

Consider a 2 layer ReLu network $H(x,\theta) = W^{(2)}\sigma(W^{(1)}x)$ with $W^{(1)} \in \mathbb{R}^{m\times n}$ and $W^{(2)} \in \mathbb{R}^m$, then for any two parameters θ_1 and θ_2 with $\mathcal{L}(\theta_i) \leq \lambda$ for $i = 1, 2$, then there is a path $\gamma(t)$ between θ_1 and θ_2 such that $\mathcal{L}(\theta_{\gamma(t)}) \leq \max(\lambda, m^{-1/n})$.

quadratic activation network: single component

Let $H(x,\theta)$ be an L layer net given by $h^{(\ell)} = \sigma(W^{(\ell)}h^{(\ell-1)})$ with $W^{(\ell)} \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$ and quadratic activation $\sigma(z) = z^2$, then once the number of parameters $n_\ell \geq 3N^{2^\ell}$ where N is the number of data entries, then the sum of squares loss function has a single connected component. For the two layer case with a single quadratic activation this simplifies to $n > 2N$.

`https://arxiv.org/pdf/1802.06384.pdf`

Hessian for two layer net (without activation)

Omitting diagonal nonlinear activation matrices.

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Let $e_{i,\mu} = \hat{y}_{i,\mu} - y_{i,\mu}$ be the error in the i^{th} entry of the output for data entry indexed by μ, and $\theta = \{W^{(1)}, W^{(2)}\} \in \mathbb{R}^{2n^2}$ be the net parameters, then the hessian of the loss function has entries

$$H_{\alpha,\beta} = \frac{\partial^2 \mathcal{L}}{\partial\theta_\alpha \partial\theta_\beta} =: H_0 + H_1$$

with positive semi-definite and error dependent components:

$$[H_0]_{\alpha,\beta} := m^{-1} \sum_{\mu=1}^{m} \sum_{i=1}^{n} \frac{\partial \hat{y}_{i,\mu}}{\partial\theta_\alpha} \frac{\partial \hat{y}_{i,\mu}}{\partial\theta_\beta} = m^{-1} [JJ^T]_{\alpha,\beta}$$

$$[H_1]_{\alpha,\beta} := m^{-1} \sum_{\mu=1}^{m} \sum_{i=1}^{n} e_{i,\mu} \frac{\partial^2 \hat{y}_{i,\mu}}{\partial\theta_\alpha \partial\theta_\beta}.$$

There are mn data entries and $2n^2$ NN parameters, with $\tau = 2n/m$ the relative over ($\tau > 1$) or under ($\tau < 1$) parameterisation.

Functions, say $\mathcal{L}$, which have hessians that are:

- positive definite (all positive eigenvalues) are convex and have a single global minima and unique minimiser,
- positive semi-definite have single global minima but non-unique minimiser due to the null-space
- indefinite (positive and negative eigenvalues) are non-convex and may be a complicated landscape with multiple local minimisers.

For the simple two layer network we considered the network has Hessian $H = H_0 + H_1$ with H_0 positive semidefinite and of size independent of the error, while H_1 is indefinite with magnitude depending on the size of $e_{i,\mu} = \hat{y}_{i,\mu} - y_{i,\mu}$.

One can interpret properties of the landscape through the Hessian by considering simplified models:

- The weights are i.i.d. random normal variable,
- The data are i.i.d. random variables,
- The residuals $e_{i,\mu} = \hat{y}_{i,\mu} - y_{i,\mu}$ are normal random variables, say $\mathcal{N}(0, 2\epsilon)$ with $\epsilon = n^{-1}\mathcal{L}$ (which also allows the gradient to vanish as $m, n \to \infty$ while m/n remains fixed; the focus is on fixed points where the gradient is zero),
- The matrices H_0 and H_1 are *freely independent* which allows us to compute the spectra of $H_0 + H_1$ from their individual spectra.

`http://proceedings.mlr.press/v70/pennington17a.html`

Wigner matrices, entries drawn $\mathcal{N}(0, \sigma^2)$, have eigenvalues drawn from the semi-circle law:

$$\rho_{sc}(\lambda) = \begin{cases} \frac{1}{2\pi\sigma^2}\sqrt{4\sigma^2 - \lambda^2} & \text{if } |\lambda| \leq 2\sigma \\ 0 & \text{otherwise} \end{cases}$$

Wishart matrices, $X = JJ^T$ product of $J \in \mathbb{R}^{n\times p}$ drawn $\mathcal{N}(0, \sigma^2/p)$ have eigenvalues drawn from the Marchenko-Pastur distribution:

$$\rho_{MP}(\lambda) = \begin{cases} \rho(\lambda) & \text{if } \tau = n/p < 1 \\ (1 - \tau^{-1})\delta(\lambda) + \rho(\lambda) & \text{otherwise} \end{cases}$$

where $\rho(\lambda) := (2\pi\lambda\sigma\tau)^{-1}\sqrt{(\lambda - \lambda_-)(\lambda_+ - \lambda)}$ for $\lambda \in [\lambda_-, \lambda_+]$ and $\lambda_\pm := \sigma(1 \pm \sqrt{\tau})^2$.

Stieltjes and $\mathcal{R}$ Transforms of probability distributions

Method to compute the spectrum under addition.

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The probability distribution of the sum of two (freely independent) random matrix distributions can be calculated using the transforms:

Stieltjes and $\mathcal{R}$ Transforms

For $z \in \mathbb{C}/\mathbb{R}$ the Stieltjes Transform, $G_\rho(z)$, of a probability distribution and its inverse are given by

$$G_\rho(z) = \int_{\mathbb{R}} \frac{\rho(t)}{z-t} dt \quad \text{and} \quad \rho(\lambda) = -\pi^{-1} \lim_{\epsilon \to 0_+} Imag(G_\rho(\lambda + i\epsilon)).$$

The Stieltjes and $\mathcal{R}$ Transform of ρ are related by the solutions of $\mathcal{R}_\rho(G_\rho(z)) + 1/G_\rho(z) = z$ and has the property that if ρ_1 and ρ_2 are freely independent then $\mathcal{R}_{\rho_1+\rho_2} = \mathcal{R}_{\rho_1} + \mathcal{R}_{\rho_2}$.

`https://terrytao.wordpress.com/tag/stieltjes-transform-method/`

Let $e_{i,\mu} = \hat{y}_{i,\mu} - y_{i,\mu}$ be the error in the i^{th} entry of the output for data entry indexed by μ, and $\theta = \{W^{(1)}, W^{(2)}\} \in \mathbb{R}^{2n^2}$ be the net parameters, then the hessian of the loss function has entries

$$H_{\alpha,\beta} = \frac{\partial^2 \mathcal{L}}{\partial\theta_\alpha \partial\theta_\beta} =: H_0 + H_1$$

with positive semi-definite and error dependent components:

$$[H_0]_{\alpha,\beta} := m^{-1} \sum_{\mu=1}^{m} \sum_{i=1}^{n} \frac{\partial \hat{y}_{i,\mu}}{\partial\theta_\alpha} \frac{\partial \hat{y}_{i,\mu}}{\partial\theta_\beta} = m^{-1}[JJ^T]_{\alpha,\beta}$$

$$[H_1]_{\alpha,\beta} := m^{-1} \sum_{\mu=1}^{m} \sum_{i=1}^{n} e_{i,\mu} \frac{\partial^2 \hat{y}_{i,\mu}}{\partial\theta_\alpha \partial\theta_\beta}.$$

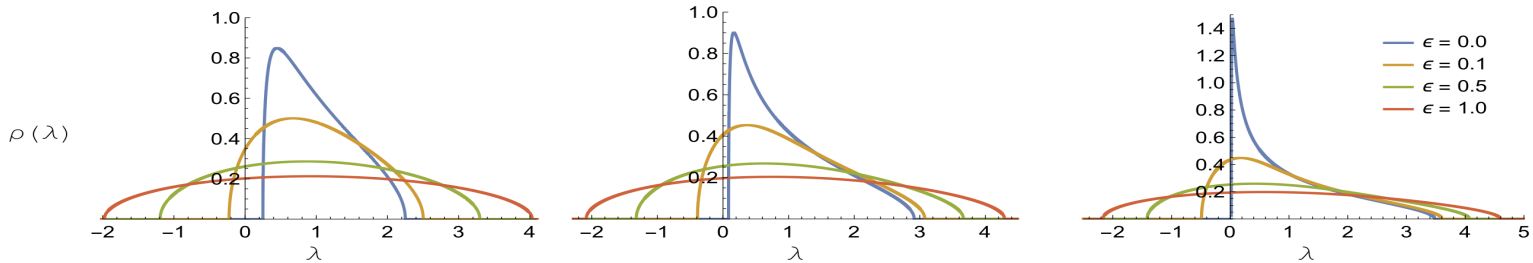
Where we assumed that H_0 and H_1 can be modelled as being drawn from Wishart and Wigner distributions respectively.

Landscape via random matrix theory (Pennington et al. 17')

Using the Pennington model ($\tau = \phi = 2n/m$ and $\epsilon = n^{-1}\mathcal{L}$) we have $\rho_{H_0}(\lambda) = \rho_{MP}(\lambda; 1, \tau)$ and $\rho_{H_1}(\lambda) = \rho_{SC}(\lambda; \sqrt{2\epsilon})$.
Their $\mathcal{R}$ transforms are respectively

$$\mathcal{R}_{H_0} = \frac{1}{1 - z\tau} \quad \text{and} \quad \mathcal{R}_{H_1} = 2\epsilon z,$$

from which follows the probability distribution, $\rho_H(\lambda; \epsilon, \tau)$:



(a) $\phi = 1/4$ (b) $\phi = 1/2$ (c) $\phi = 3/4$

Figure 1. Spectral distributions of the Wishart + Wigner approximation of the Hessian for three different ratios of parameters to data points, ϕ. As the energy ϵ of the critical point increases, the spectrum becomes more semicircular and negative eigenvalues emerge.

`http://proceedings.mlr.press/v70/pennington17a.html`

Fraction of negative eigenvalues (Pennington et al. 17')

Breakpoint dependence on ϵ_c and oversampling τ

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Consider the fraction of negative eigenvalues of $\rho_H(\lambda)$:

$$\alpha(\epsilon, \tau) := \int_{-\infty}^{0} \rho_H(\lambda; \epsilon, \tau) d\lambda.$$

Fraction of negative eigenvalues (without ReLU)

For $\rho_H(\lambda)$ modelling the Hessian of the two layer net, when α is small it is well approximated by

$$\alpha(\epsilon, \tau) \approx \alpha_0(\tau) \left| \frac{\epsilon - \epsilon_c}{\epsilon_c} \right|^{3/2}$$

where

$$\epsilon_c = \frac{1}{16}(1 - 20\tau - 8\tau^2 + (1 + 8\tau)^{3/2}).$$

`http://proceedings.mlr.press/v70/pennington17a.html`

The two layer ReLU net (Pennington et al. 17')

Now including a ReLU nonlinear activation

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The introduction of the ReLU nonlinear activation changes the Hessian, roughly setting to zero half of the entries and generating a block off-diagonal structure in H_1 with $\mathcal{R}_{H1}(z) = \frac{\epsilon\tau z}{2-\epsilon\tau^2 z^2}$.

Continuing to model H_0 as Wishart (less clear an assumption):

Fraction of negative eigenvalues (with ReLU)

For $\rho_H(\lambda)$ modelling the Hessian of the two layer net, when α is small it is well approximated by

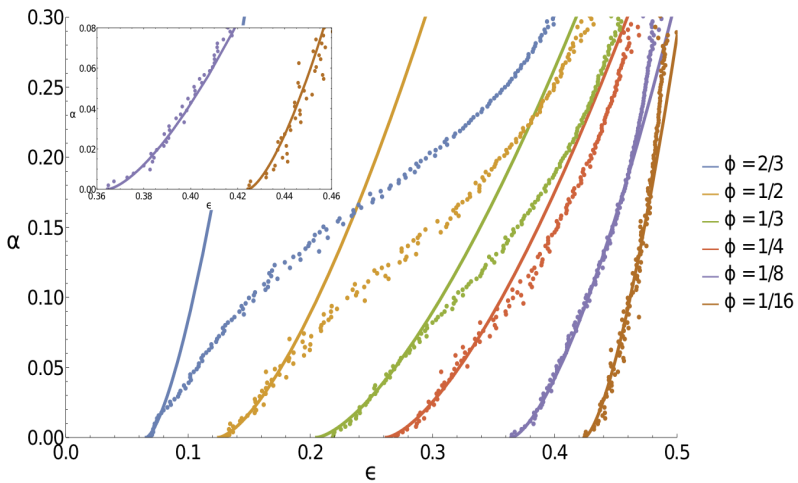
$$\alpha(\epsilon,\tau) \approx \tilde{\alpha}_0(\tau) \left| \frac{\epsilon - \epsilon_c}{\epsilon_c} \right|^{3/2} \quad \text{where}$$

$$\epsilon_c = \frac{\sigma^2(27 - 18\xi - \xi^2 + 8\xi^{3/2})}{32\tau(1-\tau)^3}, \quad \text{with} \quad \xi = 1 + 16\tau - 8\tau^2.$$

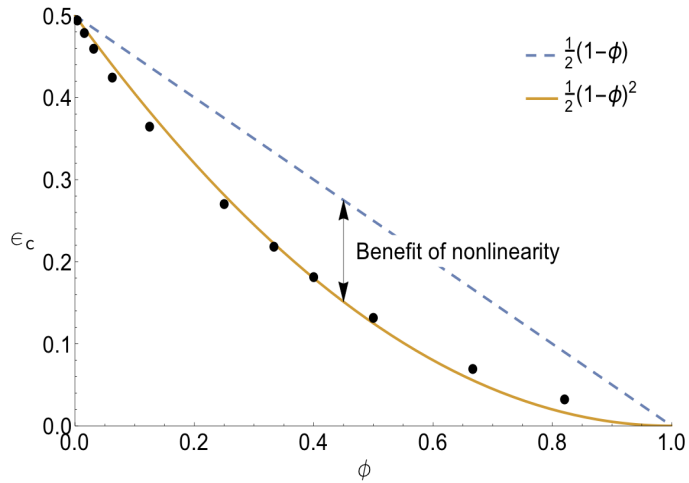
`http://proceedings.mlr.press/v70/pennington17a.html`

Empirical values of ϵ_c and α (Pennington et al. 17')

Match of empirical and analytical calculations



(a) Index of critical points versus energy



(b) Energy of minimizers versus parameters/data points

Figure 6. Empirical observations of the distribution of critical points in single-hidden-layer $\tanh$ networks with varying ratios of parameters to data points, ϕ. (a) Each point represents the mean energy of critical points with index α, averaged over ~200 training runs. Solid lines are best fit curves for small $\alpha \approx \alpha_0|\epsilon - \epsilon_c|^{3/2}$. The good agreement (emphasized in the inset, which shows the behavior for small α) provides support for our theoretical prediction of the $3/2$ scaling. (b) The best fit value of ϵ_c from (a) versus ϕ. A surprisingly good fit is obtained with $\epsilon_c = \frac{1}{2}(1-\phi)^2$. Linear networks obey $\epsilon_c = \frac{1}{2}(1-\phi)$. The difference between the curves shows the benefit obtained from using a nonlinear activation function.

http://proceedings.mlr.press/v70/pennington17a.html

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Dimension of global minimizer submanifold

Let $H(x;\theta)$ be a DNN from $\mathbb{R}^n$ to $\mathbb{R}^r$ with smooth nonlinear activation $\phi(\cdot)$, let the loss function over d distinct data elements be defined as

$$\mathcal{L} = (2m)^{-1} \sum_{\mu=1}^{d} \|H(x_\mu;\theta) - y_\mu)\|_2^2,$$

and let $\Omega^*_{\mathcal{L}}(0) = \{\theta : \ \mathcal{L}(\theta; X, Y) = 0\}$ be the set of weight and bias trainable parameters for which the DNN exactly fits the d data elements. Then, subject to possibly arbitrarily small perturbation, the set $\Omega^*_{\mathcal{L}}(0)$ is a smooth $(d - rn)-$dimensional submanifold (possibly empty) of $\mathbb{R}^d$.

https://epubs.siam.org/doi/pdf/10.1137/19M1308943

DNN loss landscape summary

Structure of the loss landscape dimensionality dependence

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- Loss landscapes for DNNs can be non-convex and hence difficult to optimise.
- The number of components of a loss landscape level curve can be analysed, and in some settings has a single component greatly aiding its optimisation.
- Increasing width of a DNN can improve the loss landscape.
- The local shape of random nets can be analysed, showing that when near a minima the Hessian has only non-negative eigenvalues.
- When the amount of data exceeds the product of the input and output dimensions, DNNs with smooth non-linear activations which exactly fit the data, have smooth manifold of a known dimension.