Linearized Networks

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This is some derivations in paper Wide Neural Networks of Any Depth Evolve as Linear Models Under Gradient Descent[1].

1 Problem Setup

Training set: $D \subseteq \mathbb{R}^{n_0 \times n_k}$, $\mathcal{X} = \{x : (x, y) \in D\}$, $\mathcal{Y} = \{y : (x, y) \in D\}$.

Consider a fully-connected feed-forward network with L hidden layers with widths n_l , for l = 1, ..., L and readout layer $n_{L+1} = k$.

$$\begin{cases}
h^{l+1} = x^l W^{l+1} + b^{l+1} \\
x^{l+1} = \phi(x^l)
\end{cases}
\begin{cases}
W_{ij}^{l+1} = \frac{\sigma_{\omega}}{\sqrt{n_l}} w_{ij}^{l+1} \\
b_j^l = \sigma_b \beta_j^l
\end{cases}$$
(1)

$$f_t(x) \equiv h^{L+1}(x) \in \mathbb{R}^k \tag{2}$$

where $W^{l+1} \in \mathbb{R}^{n_l \times n_{l+1}}, b^{l+1} \in \mathbb{R}^{n_{l+1}}, w_{i,j}^l, \beta_j^l \sim \mathcal{N}(0,1)$

$$\nabla_{\theta} f_{t}(\mathcal{X}) = \begin{bmatrix} \nabla_{\theta} f_{1}(x_{1}) \\ \vdots \\ \nabla_{\theta} f_{k}(x_{1}) \\ \vdots \\ \nabla_{\theta} f_{1}(x_{|D|}) \\ \vdots \\ \nabla_{\theta} f_{k}(x_{|D|}) \end{bmatrix} = \begin{bmatrix} \nabla_{\theta_{1}} f_{1}(x_{1}) & \cdots & \nabla_{\theta_{|\theta|}} f_{1}(x_{1}) \\ \vdots & \ddots & \vdots \\ \nabla_{\theta_{1}} f_{k}(x_{1}) & \cdots & \nabla_{\theta_{|\theta|}} f_{k}(x_{1}) \\ \vdots & \ddots & \vdots \\ \nabla_{\theta_{1}} f_{1}(x_{|D|}) & \cdots & \nabla_{\theta_{|\theta|}} f_{1}(x_{|D|}) \\ \vdots & \ddots & \vdots \\ \nabla_{\theta_{1}} f_{k}(x_{|D|}) & \cdots & \nabla_{\theta_{|\theta|}} f_{k}(x_{|D|}) \end{bmatrix} \in \mathbb{R}^{k|D| \times |\theta|}$$

$$(3)$$

where $f_t(\mathcal{X}) = vec([f_t(x)]_{x \in \mathcal{X}}) \in \mathbb{R}^{k|D| \times 1}$

Empirical Tangent Kernel:

$$\hat{\Theta}_{t} \equiv \hat{\Theta}_{t}(\mathcal{X}, \mathcal{X}) = \nabla_{\theta} f_{t}(\mathcal{X}) f_{t}(\mathcal{X})^{T} \\
= \begin{bmatrix}
\nabla_{\theta} f_{1}(x_{1}) \nabla_{\theta} f_{1}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{1}(x_{1}) \nabla_{\theta} f_{k}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{1}(x_{1}) \nabla_{\theta} f_{1}(x_{|D|})^{T} & \cdots & \nabla_{\theta} f_{1}(x_{1}) \nabla_{\theta} f_{k}(x_{|D|})^{T} \\
\vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\nabla_{\theta} f_{k}(x_{1}) \nabla_{\theta} f_{1}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{1}) \nabla_{\theta} f_{k}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{1}) \nabla_{\theta} f_{1}(x_{|D|})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{1}) \nabla_{\theta} f_{k}(x_{|D|})^{T} \\
\vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\nabla_{\theta} f_{1}(x_{|D|}) \nabla_{\theta} f_{1}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{1}(x_{|D|}) \nabla_{\theta} f_{k}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{1}(x_{|D|}) \nabla_{\theta} f_{1}(x_{|D|})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{|D|})^{T} \\
\vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\nabla_{\theta} f_{k}(x_{|D|}) \nabla_{\theta} f_{1}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{|D|}) \nabla_{\theta} f_{k}(x_{1})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{|D|}) \nabla_{\theta} f_{1}(x_{|D|})^{T} & \cdots & \nabla_{\theta} f_{k}(x_{|D|}) \nabla_{\theta} f_{k}(x_{|D|})^{T} \end{bmatrix}$$

$$= \begin{bmatrix} \hat{\Theta}_{t}(x_{1}, \mathcal{X}) \\ \vdots \\ \hat{\Theta}_{t}(x_{|D|}, \mathcal{X}) \end{bmatrix} \in \mathbb{R}^{k|D| \times k|D|}$$

Continuous time gradient descent:

$$\dot{\theta}_t = -\eta \nabla_{\theta} f_t(\mathcal{X})^T \nabla_{f_t(\mathcal{X})} \mathcal{L} \in \mathbb{R}^{|\theta| \times 1}$$
(5)

(4)

$$\dot{f}_t(\mathcal{X}) = \nabla_{\theta} f_t(\mathcal{X}) \dot{\theta}_t = -\eta \nabla_{\theta} f_t(\mathcal{X}) \nabla_{\theta} f_t(\mathcal{X})^T \nabla_{f_t(\mathcal{X})} \mathcal{L} = -\eta \hat{\Theta}_t(\mathcal{X}, \mathcal{X}) \nabla_{f_t(\mathcal{X})} \mathcal{L}$$
(6)

In the case of an MSE loss, i.e., $\ell(\hat{y}, y) = \frac{1}{2} ||\hat{y} - y||_2^2$,

$$\nabla_{f_t(\mathcal{X})} \mathcal{L} = f_t(\mathcal{X}) - \mathcal{Y} \in \mathbb{R}^{k|D| \times 1}$$
(7)

$$\dot{f}_t(\mathcal{X}) = -\eta \hat{\Theta}_t(\mathcal{X}, \mathcal{X}) (f_t(\mathcal{X}) - \mathcal{Y}) \tag{8}$$

which a first-order system of linear differential equations or a matrix differential equation.

When $\hat{\Theta}_t(\mathcal{X}, \mathcal{X}) \to \Theta$ is a constant matrix, the solution is given by

$$f_t(\mathcal{X}) = e^{-\eta \Theta t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$

= $(I - e^{-\eta \Theta t})\mathcal{Y} + e^{-\eta \Theta t} f_0(\mathcal{X})$ (9)

where $e^X = \sum_{k=0}^{\infty} \frac{1}{k!} X^k$. There is no closed-form solution for the differential equations when $\hat{\Theta}_t(\mathcal{X}, \mathcal{X})$ is varing with time, one has to use either a numerical method, or an approximation method such as Magnus expansion.

2 Linearized Model

$$f_t^{lin}(x) \equiv f_0(x) + \nabla_{\theta} f_0(x)|_{\theta = \theta_0} \ \omega_t, \quad \omega_t \equiv \theta_t - \theta_0 \tag{10}$$

$$\nabla_{\theta} f_t^{lin}(x) = 0 + \nabla_{\theta} f_0(x)|_{\theta = \theta_0} = \nabla_{\theta} f_0(x) \tag{11}$$

$$\dot{\omega}_t = \dot{\theta}_t = -\eta \nabla_{\theta} f_t^{lin}(\mathcal{X})^T \nabla_{f_t^{lin}(\mathcal{X})} \mathcal{L}$$
$$= -\eta \nabla_{\theta} f_0(\mathcal{X})^T \nabla_{f_t^{lin}(\mathcal{X})} \mathcal{L}$$
(12)

$$\dot{f}_{t}^{lin}(\mathcal{X}) = \nabla_{\theta} f_{t}^{lin}(\mathcal{X}) \dot{\theta}_{t} = -\eta \nabla_{\theta} f_{t}^{lin}(\mathcal{X}) \nabla_{\theta} f_{t}^{lin}(\mathcal{X})^{T} \nabla_{f_{t}^{lin}(\mathcal{X})} \mathcal{L}
= -\eta \nabla_{\theta} f_{0}(x) \nabla_{\theta} f_{0}(x)^{T} \nabla_{f_{t}^{lin}(\mathcal{X})} \mathcal{L} = -\eta \hat{\Theta}_{0}(\mathcal{X}, \mathcal{X}) \nabla_{f_{t}^{lin}(\mathcal{X})} \mathcal{L}$$
(13)

Note that (13) is identical to (6) if tangent kernel is deterministic during training, i.e. $\hat{\Theta}_t(\mathcal{X}, \mathcal{X}) = \hat{\Theta}_0(\mathcal{X}, \mathcal{X})$.

In the case of an MSE loss,

$$\dot{f}_t^{lin}(\mathcal{X}) = -\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X}) \left(f_t^{lin}(\mathcal{X}) - \mathcal{Y} \right)$$
(14)

Since $\hat{\Theta}_0(\mathcal{X}, \mathcal{X})$ is a constant matrix, (14) has a solution like (9)

$$f_t^{lin}(\mathcal{X}) = e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$
(15)

Take this into equation (12)

$$\dot{\omega}_t = -\eta \nabla_{\theta} f_0(\mathcal{X})^T \left(f_t^{lin}(\mathcal{X}) - \mathcal{Y} \right)$$

$$= -\eta \nabla_{\theta} f_0(\mathcal{X})^T e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \left(f_0(\mathcal{X}) - \mathcal{Y} \right)$$
(16)

Integrate over time,

$$\int_{0}^{t} e^{-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t} dt = \int_{0}^{t} \sum_{k=0}^{\infty} \frac{1}{k!} (-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t)^{k} dt$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} (-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t)^{k} \frac{t}{k+1}$$

$$= -\frac{1}{\eta} \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})^{-1} \sum_{k=0}^{\infty} \frac{1}{(k+1)!} (-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t)^{k+1}$$

$$= -\frac{1}{\eta} \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})^{-1} \sum_{k=1}^{\infty} \frac{1}{k!} (-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t)^{k}$$

$$= -\frac{1}{\eta} \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})^{-1} \left(e^{-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t} - I \right)$$

$$= \frac{1}{\eta} \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})^{-1} \left(I - e^{-\eta \hat{\Theta}_{0}(\mathcal{X},\mathcal{X})t} \right)$$

$$\omega_t = -\nabla_{\theta} f_0(\mathcal{X})^T \hat{\Theta}_0(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \Big) \Big(f_0(\mathcal{X}) - \mathcal{Y} \Big)$$
(18)

Take this into equation (10), we get

$$f_t^{lin}(x) = f_0(x) + \nabla_{\theta} f_0(x)|_{\theta=\theta_0} \omega_t$$

$$= f_0(x) - \nabla_{\theta} f_0(x) \nabla_{\theta} f_0(\mathcal{X})^T \hat{\Theta}_0(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \Big) \Big(f_0(\mathcal{X}) - \mathcal{Y} \Big)$$

$$= f_0(x) - \hat{\Theta}_0(x, \mathcal{X}) \hat{\Theta}_0(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \Big) \Big(f_0(\mathcal{X}) - \mathcal{Y} \Big)$$

$$= \hat{\Theta}_0(x, \mathcal{X}) \hat{\Theta}_0(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \Big) \mathcal{Y}$$

$$+ f_0(x) - \hat{\Theta}_0(x, \mathcal{X}) \hat{\Theta}_0(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} \Big) f_0(\mathcal{X})$$

$$(19)$$

3 Infinite width limit yields a Gaussian process

Let

$$\mathcal{K}^{i,j}(x,x') = \lim_{\min(n_1,\dots,n_L) \to \infty} \mathbb{E}[f_0^i(x)f_0^j(x')]$$
 (20)

denotes the covariance between the *i*-th output of x and j-th output of x' at initialization. Then $f_0(\mathcal{X}) \sim \mathcal{N}(0, \mathcal{K}(\mathcal{X}, \mathcal{X}))$, i.e.

$$p(f(\mathcal{X})|\mathcal{X}) = \mathcal{N}(0, \mathcal{K}(\mathcal{X}, \mathcal{X}))$$
(21)

For a test input $x \in \mathcal{X}_T$, the joint output distribution $f([x,\mathcal{X}])$ is also multivariate Gaussian, whose covariance matrix is

$$\mathbf{K} = \begin{bmatrix} \mathcal{K}(\mathcal{X}, \mathcal{X}) & \mathcal{K}(x, \mathcal{X})^T \\ \mathcal{K}(x, \mathcal{X}) & \mathcal{K}(x, x) \end{bmatrix}$$
 (22)

That is

$$p(f(x), f(\mathcal{X})|x, \mathcal{X}) = \mathcal{N}(0, \mathbf{K})$$
(23)

We have to predict the probability distribution of f(x), conditioning on the training samples, $f(\mathcal{X}) = \mathcal{Y}$, i.e. $p(f(\mathcal{X}) = \mathcal{Y} | \mathcal{X}, \mathcal{Y}) = 1$.

$$p(f(x)|x,\mathcal{X},\mathcal{Y}) = p(f(x)|x,\mathcal{X},f(\mathcal{X}))$$

$$= \frac{p(f(x),x,\mathcal{X},f(\mathcal{X}))}{p(x,\mathcal{X},f(\mathcal{X}))}$$

$$= \frac{p(f(x),f(\mathcal{X})|x,\mathcal{X})p(x,\mathcal{X})}{p(x,\mathcal{X},f(\mathcal{X}))}$$

$$= \frac{p(f(x),f(\mathcal{X})|x,\mathcal{X})}{p(f(\mathcal{X})|x,\mathcal{X})}$$

$$= \frac{p(f(x),f(\mathcal{X})|x,\mathcal{X})}{p(f(\mathcal{X})|\mathcal{X})}$$

$$= \frac{p(f(x),f(\mathcal{X})|x,\mathcal{X})}{p(f(\mathcal{X})|\mathcal{X})}$$

$$= \frac{\mathcal{N}(0,\mathbf{K})}{\mathcal{N}(0,\mathcal{K}(\mathcal{X},\mathcal{X}))}$$
(24)

This is also a gaussian distribution given by

$$\mu(x) = \mathcal{K}(x, \mathcal{X})\mathcal{K}(\mathcal{X}, \mathcal{X})^{-1}\mathcal{Y}$$
(25)

$$\Sigma(x) = \mathcal{K}(x, x) - \mathcal{K}(x, x)\mathcal{K}(x, x)^{-1}\mathcal{K}(x, x)^{T}$$
(26)

This corresponds to only the readout layer $n_{L+1} = k$ is being trained (see [1] appendix D).

4 Corollary 1

In the infinite width setting, $[f_0(x), f_0(\mathcal{X})]$ is Gaussian distributed and $\hat{\Theta}_0$ converges in probability to a deterministic kernel Θ . For any t, (19) is Gaussian distributed because it describe an affine transform of the Gaussian $[f_0(x), f_0(\mathcal{X})]$.

$$\mathbb{E}[f_t^{lin}(x)] = \mathbb{E}[\Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\mathcal{Y}]$$

$$+ \mathbb{E}[f_0(x)] - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\mathbb{E}[f_0(\mathcal{X})]$$

$$= \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\mathcal{Y}$$

$$(27)$$

$$\begin{split} &\Sigma(x,x) = \mathbb{E}[f_t^{lin}(x)f_t^{lin}(x)^T] \\ &= \mathbb{E}\big[[f_0(x) - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)] \\ &\quad [f_0(x) - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)]^T\big] \\ &= \mathbb{E}\big[[f_0(x) - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)] \\ &\quad [f_0(x)^T - \big(f_0(\mathcal{X}) - \mathcal{Y}\big)^T\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x)]\big] \\ &= \mathbb{E}\big[f_0(x)f_0(x)^T - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)f_0(x)^T \\ &\quad - f_0(x)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)^T\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x) \\ &\quad + \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\big(f_0(\mathcal{X}) - \mathcal{Y}\big)\Big(f_0(\mathcal{X}) - \mathcal{Y}\big)^T\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x) \\ &\quad = \mathcal{K}(x,x) - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\mathcal{K}(\mathcal{X},x) - \mathcal{K}(x,\mathcal{X})\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x) \\ &\quad + \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\mathcal{K}(\mathcal{X},\mathcal{X})\Big(I - e^{-\eta\Theta(\mathcal{X},\mathcal{X})t}\Big)\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x) \end{aligned}$$

When $t \to \infty$, $e^{-\eta\Theta(\mathcal{X},\mathcal{X})t} \to \mathbf{0}$,

$$\mathbb{E}[f_t^{lin}(x)] = \Theta(x, \mathcal{X})\Theta(\mathcal{X}, \mathcal{X})^{-1}\mathcal{Y}$$
(29)

$$\Sigma(x,x) = \mathcal{K}(x,x) - \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\mathcal{K}(\mathcal{X},x) - \mathcal{K}(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x) + \Theta(x,\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\mathcal{K}(\mathcal{X},\mathcal{X})\Theta(\mathcal{X},\mathcal{X})^{-1}\Theta(\mathcal{X},x)$$
(30)

5 Gradient flow dynamics for training only the readout-layer

This is appendix D in paper[1].

$$f(x) = \overline{x}(x)\theta^{L+1} = [\overline{x}(x) \cdot \theta_1^{L+1}, \cdots, \overline{x}(x) \cdot \theta_i^{L+1}, \cdots, \overline{x}(x) \cdot \theta_k^{L+1}]$$
(31)

$$\overline{x}(x) = \left[\frac{\sigma_{\omega} x^{L}(x)}{\sqrt{n_{l}}}, \sigma_{b}\right] \in \mathbb{R}^{n_{L}+1}, \quad \theta^{L+1} = \begin{bmatrix} W^{L+1} \\ b^{L+1} \end{bmatrix} \in \mathbb{R}^{(n_{L}+1) \times k}$$
(32)

where θ_i^{L+1} is the i_{th} column of θ^{L+1} . Note $n_{L+1} = k$.

$$\hat{\mathcal{K}}(x, x') = \mathbb{E}[f_0^i(x) \cdot f_0^i(x')] = \mathbb{E}[\overline{x}(x) \cdot \theta_i^{L+1} \cdot \overline{x}(x') \cdot \theta_i^{L+1}]
= \overline{x}(x) \cdot \overline{x}(x') = \frac{\sigma_\omega^2}{n_l} x^L(x) \cdot x^L(x') + \sigma_b^2 \to \mathcal{K}(x, x')$$
(33)

$$\nabla_{\theta^{L+1}} f(x) = \begin{bmatrix} \nabla_{\theta^{L+1}} f_1(x) \\ \vdots \\ \nabla_{\theta^{L+1}} f_k(x) \end{bmatrix} = \begin{bmatrix} \overline{x}(x), & \mathbf{0}, & \cdots, & \mathbf{0}, & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}, & \mathbf{0}, & \cdots, & \mathbf{0}, & \overline{x}(x) \end{bmatrix} \in \mathbb{R}^{k \times (n_L + 1)k}$$
(34)

$$\nabla_{\theta^{L+1}} f(\mathcal{X}) = \begin{bmatrix} \nabla_{\theta^{L+1}} f_1(x_1) \\ \vdots \\ \nabla_{\theta^{L+1}} f_k(x_1) \\ \vdots \\ \nabla_{\theta^{L+1}} f_1(x_{|D|}) \\ \vdots \\ \nabla_{\theta^{L+1}} f_k(x_{|D|}) \end{bmatrix} = \begin{bmatrix} \overline{x}(x_1), & \mathbf{0}, & \cdots, & \mathbf{0}, & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}, & \mathbf{0}, & \cdots, & \mathbf{0}, & \overline{x}(x_1) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \overline{x}(x_{|D|}), & \mathbf{0}, & \cdots, & \mathbf{0}, & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}, & \mathbf{0}, & \cdots, & \mathbf{0}, & \overline{x}(x_{|D|}) \end{bmatrix} \in \mathbb{R}^{k|D| \times (n_L + 1)k}$$
(35)

In the case of MSE loss,

$$\mathcal{L} = \frac{1}{2} \| f(\mathcal{X}) - \mathcal{Y} \|_{2}^{2} = \frac{1}{2} \| \overline{x}(\mathcal{X}) \theta^{L+1} - \mathcal{Y} \|_{2}^{2}$$
(36)

$$\dot{\theta}^{L+1} = -\eta \nabla_{\theta^{L+1}} f(\mathcal{X})^T \nabla_{f_t(\mathcal{X})} \mathcal{L} = -\eta \nabla_{\theta^{L+1}} f(\mathcal{X})^T (\overline{x}(\mathcal{X}) \theta^{L+1} - \mathcal{Y})$$

$$= -\eta \begin{bmatrix} \overline{x}(x_1)^T, & \cdots & \mathbf{0}, & \cdots, & \overline{x}(x_{|D|})^T, & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{0}, & \cdots & \overline{x}(x_1)^T, & \cdots, & \mathbf{0}, & \cdots & \overline{x}(x_{|D|})^T \end{bmatrix} \begin{bmatrix} \overline{x}(x_1)\theta_1^{L+1} - y_{1,1} \\ \vdots \\ \overline{x}(x_1)\theta_k^{L+1} - y_{1,k} \\ \vdots \\ \overline{x}(x_{|D|})\theta_k^{L+1} - y_{|D|,1} \\ \vdots \\ \overline{x}(x_{|D|})\theta_k^{L+1} - y_{|D|,k} \end{bmatrix}$$
(37)

Since different dimension of outputs are independent, we consider only one output,

$$\dot{\theta}^{L+1} = -\eta \nabla_{\theta^{L+1}} f(\mathcal{X})^T \nabla_{f_t(\mathcal{X})} \mathcal{L} = -\eta \nabla_{\theta^{L+1}} f(\mathcal{X})^T (\overline{x}(\mathcal{X}) \theta^{L+1} - \mathcal{Y})
= -\eta \overline{x}(\mathcal{X})^T (\overline{x}(\mathcal{X}) \theta^{L+1} - \mathcal{Y})$$
(38)

Since $\overline{x}(\mathcal{X})^T \overline{x}(\mathcal{X})$ is a constant matrix, we can get the result as

$$\overline{x}(\mathcal{X})\theta_t^{L+1} = e^{-\eta \overline{x}(\mathcal{X})^T \overline{x}(\mathcal{X})t} (\overline{x}(\mathcal{X})\theta_0^{L+1} - \mathcal{Y}) + \mathcal{Y}$$
(39)

$$f_t(\mathcal{X}) = e^{-\eta \overline{x}(\mathcal{X})^T \overline{x}(\mathcal{X})t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$
(40)

When we only train the readout-layer, the original network and its linearization are identical. Compare with (15),

$$f_t(\mathcal{X}) = e^{-\eta \overline{x}(\mathcal{X})^T \overline{x}(\mathcal{X})t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$

$$= e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$
(41)

We can see

$$\overline{x}(\mathcal{X})^T \overline{x}(\mathcal{X}) = \hat{\Theta}_0(\mathcal{X}, \mathcal{X}) = \hat{\mathcal{K}}(\mathcal{X}, \mathcal{X}) \tag{42}$$

Take this into (19)

$$f_t(x) = f_0(x) - \hat{\mathcal{K}}(x, \mathcal{X})\hat{\mathcal{K}}(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \hat{\mathcal{K}}(\mathcal{X}, \mathcal{X})t} \Big) \Big(f_0(\mathcal{X}) - \mathcal{Y} \Big)$$
(43)

In the infinite width setting, $\hat{\mathcal{K}} \to \mathcal{K}$, and $\Theta = \mathcal{K}$. Take this into the results of Corollary 1,

$$\mathbb{E}[f_t(x)] = \mathcal{K}(x, \mathcal{X})\mathcal{K}(\mathcal{X}, \mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t} \Big) \mathcal{Y}$$
(44)

$$\Sigma(x,x) = \mathcal{K}(x,x) - \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},x) - \mathcal{K}(x,\mathcal{X}) \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},x)^{-1} \mathcal{K}(\mathcal{X},x)$$

$$+ \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},\mathcal{X}) \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \mathcal{K}(\mathcal{X},x)$$

$$= \mathcal{K}(x,x) - 2\mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},x)$$

$$+ \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},\mathcal{X}) \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \mathcal{K}(\mathcal{X},x)$$

$$(45)$$

where

$$\left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right) \mathcal{K}(\mathcal{X}, \mathcal{X}) \left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right) \mathcal{K}(\mathcal{X}, \mathcal{X})^{-1}
= \left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right) \mathcal{K}(\mathcal{X}, \mathcal{X}) \mathcal{K}(\mathcal{X}, \mathcal{X})^{-1} \left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right)
= \left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right) \left(I - e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}\right)
= I - 2e^{-\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t} + e^{-2\eta \mathcal{K}(\mathcal{X}, \mathcal{X})t}$$
(46)

Take this into the equation,

$$\Sigma(x,x) = \mathcal{K}(x,x) - 2\mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},x)$$

$$+ \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - 2e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} + e^{-2\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(\mathcal{X},x)$$

$$= \mathcal{K}(x,x) + \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} - I \Big) \mathcal{K}(\mathcal{X},x)$$

$$= \mathcal{K}(x,x) - \mathcal{K}(x,\mathcal{X})\mathcal{K}(\mathcal{X},\mathcal{X})^{-1} \Big(I - e^{-\eta \mathcal{K}(\mathcal{X},\mathcal{X})t} \Big) \mathcal{K}(x,\mathcal{X})^{T}$$

$$(47)$$

6 Infinite width networks are linearized networks

Theorem 2.1 (informal). Let $n_1 = \cdots = n_L = n$ and assume $\lambda_{min}(\Theta) > 0$. Applying gradient descent with learning rate $\eta < \eta_{critical}$ (or gradient flow), for every $x \in \mathbb{R}^{n_0}$ with $||x||_2 \leq 1$, with probability arbitrarily close to 1 over random initialization,

$$\sup_{t>0} \|f_t(x) - f_t^{lin}(x)\|_2, \ \sup_{t>0} \frac{\|\theta_t - \theta_0\|_2}{\sqrt{n}}, \ \sup_{t>0} \|\hat{\Theta}_t - \hat{\Theta}_0\|_F = \mathcal{O}(n^{-\frac{1}{2}}), \ as \quad n \to \infty$$
 (48)

Some short-hand notations:

$$f(\theta_t) = f(\mathcal{X}, \theta_t) \in \mathbb{R}^{|\mathcal{X}|k} \tag{49}$$

$$g(\theta_t) = g(\mathcal{X}, \theta_t) - \mathcal{Y} \in \mathbb{R}^{|\mathcal{X}|k}$$
(50)

$$J(\theta_t) = \nabla f(\theta_t) \in \mathbb{R}^{(|\mathcal{X}|k) \times |\theta|}$$
(51)

$$\begin{cases} \hat{\Theta}_t := \hat{\Theta}_t(\mathcal{X}, \mathcal{X}) = \frac{1}{n} J(\theta_t) J(\theta_t)^T \\ \Theta := \lim_{n \to \infty} \hat{\Theta}_0 \quad \text{in probability.} \end{cases}$$
 (52)

The gradient descent update with learning rate η :

$$\theta_{t+1} = \theta_t - \eta J(\theta_t)^T g(\theta_t) \tag{53}$$

Lemma 1 (Local Lipschitzness of the Jacobian). There is a K > 0 such that for every C > 0, with high probability over random initialization (w.h.p.o.r.i.) the following holds

$$\begin{cases}
\frac{1}{\sqrt{n}} \left\| J(\theta) - J(\tilde{\theta}) \right\|_{F} & \leq K \left\| \theta - \tilde{\theta} \right\|_{2} \\
\frac{1}{\sqrt{n}} \left\| J(\theta) \right\|_{F} & \leq K
\end{cases}, \quad \forall \theta, \tilde{\theta} \in B(\theta_{0}, Cn^{-\frac{1}{2}}) \tag{54}$$

where

$$B(\theta_0, R) := \{\theta : \|\theta - \theta_0\|_2 < R\}$$
(55)

Theorem G.1 (Gradient descent). Assume **Assumptions [1-4]**. For $\delta_0 > 0$ and $\eta_0 < \eta_{critical}$, there exist $R_0 > 0$, $N \in \mathbb{N}$ and K > 1, such that for every $n \geq N$, the following holds with probability at least $(1 - \delta_0)$ over random initialization when applying gradient descent with learning rate $\eta = \frac{\eta_0}{n}$,

$$\begin{cases}
\|g(\theta_t)\|_2 \le (1 - \frac{\eta_0 \lambda_{min}}{3})^t R_0 \\
\sum_{j=1}^t \|\theta_j - \theta_{j-1}\|_2 \le \frac{\eta_0 K R_0}{\sqrt{n}} \sum_{j=1}^t (1 - \frac{\eta_0 \lambda_{min}}{3})^{j-1} \le \frac{3K R_0}{\lambda_{min}} n^{-\frac{1}{2}}
\end{cases}$$
(56)

and

$$\sup_{t} \left\| \hat{\Theta}_0 - \hat{\Theta}_t \right\|_F \le \frac{6K^3 R_0}{\lambda_{min}} n^{-\frac{1}{2}} \tag{57}$$

The first inequation of (56) indicates when $t \to \infty$, $g(\theta_t) \to 0$, i.e. the convergence of training. The second inequation of (56) bounds the change of θ with n. The larger n is, the less θ changes. The inequation of (57) bounds the change of $\hat{\Theta}$ with n during training.

6.1 Proof of Theorem G.1

We first prove (56) by induction.

Since $f(x_0)$ and $g(x_0)$ are gaussian distributed, for arbitrarily small $\delta_0 > 0$, there exist R_0 and n_0 (both may depend on $\delta_0, |\mathcal{X}|$ and \mathcal{K}) such that for every $n \geq n_0$, with probability at least $(1 - \delta_0)$ over random initialization,

$$||g(\theta_0)||_2 < R_0 \tag{58}$$

This is the case of t = 0 for (56). Assume (56) holds for t = t. Then for t + 1

$$\|\theta_{t+1} - \theta_t\|_2 = \|-\eta J(\theta_t)^T g(\theta_t)\|_2 \le \eta \|J(\theta_t)\|_{op} \|g(\theta_t)\|_2 \le \frac{\eta_0}{n} \|J(\theta_t)\|_{op} \left(1 - \frac{\eta_0 \lambda_{min}}{3}\right)^t R_0$$
 (59)

Here the $\|\cdot\|_{op}$ is the induced 2-norm for a matrix. From Lemma 1 and the property of matrix norm,

$$||J(\theta_t)||_2 = \sigma_{max}(J(\theta_t)) \le ||J(\theta_t)||_E \le K\sqrt{n}$$

$$\tag{60}$$

So we get

$$\|\theta_{t+1} - \theta_t\|_2 \le \frac{K\eta_0}{\sqrt{n}} \left(1 - \frac{\eta_0 \lambda_{min}}{3}\right)^t R_0$$
 (61)

Then

$$\|\theta_{t+1} - \theta_{0}\|_{2} = \|\theta_{t+1} - \theta_{t} + \theta_{t} - \theta_{t-1} + \dots - \theta_{0}\|_{2}$$

$$\leq \|\theta_{t+1} - \theta_{t}\|_{2} + \dots + \|\theta_{1} - \theta_{0}\|_{2}$$

$$\leq \sum_{i=1}^{t+1} \frac{K\eta_{0}R_{0}}{\sqrt{n}} \left(1 - \frac{\eta_{0}\lambda_{min}}{3}\right)^{j-1}$$
(62)

which is the sum of a geometric progression.

$$\sum_{j=1}^{t+1} \left(1 - \frac{\eta_0 \lambda_{min}}{3} \right)^{j-1} = \frac{1 - \left(1 - \frac{\eta_0 \lambda_{min}}{3} \right)^{t+1}}{1 - \left(1 - \frac{\eta_0 \lambda_{min}}{3} \right)} = 3 \frac{1 - \left(1 - \frac{\eta_0 \lambda_{min}}{3} \right)^{t+1}}{\eta_0 \lambda_{min}} \le \frac{3}{\eta_0 \lambda_{min}}$$
(63)

So we get the second inequation of (56).

$$\|\theta_{t+1} - \theta_0\|_2 \le \sum_{j=1}^{t+1} \|\theta_j - \theta_{j-1}\|_2 \le \sum_{j=1}^{t+1} \frac{K\eta_0 R_0}{\sqrt{n}} \left(1 - \frac{\eta_0 \lambda_{min}}{3}\right)^{j-1} \le \frac{K\eta_0 R_0}{\sqrt{n}} \frac{3}{\eta_0 \lambda_{min}} = \frac{3KR_0}{\lambda_{min}} n^{-\frac{1}{2}}$$
 (64)

For the first inequation of (56), we apply the mean value theorem.

$$||g(\theta_{t+1})||_{2} = ||g(\theta_{t+1}) - g(\theta_{t}) + g(\theta_{t})||_{2}$$

$$= ||J(\tilde{\theta}_{t})(\theta_{t+1} - \theta_{t}) + g(\theta_{t})||_{2}$$

$$= ||-\eta J(\tilde{\theta}_{t})J(\theta_{t})^{T}g(\theta_{t}) + g(\theta_{t})||_{2}$$

$$= ||(I - \eta J(\tilde{\theta}_{t})J(\theta_{t})^{T})g(\theta_{t})||_{2}$$

$$\leq ||I - \eta J(\tilde{\theta}_{t})J(\theta_{t})^{T}||_{op} ||g(\theta_{t})||_{2}$$

$$\leq ||I - \eta J(\tilde{\theta}_{t})J(\theta_{t})^{T}||_{op} (1 - \frac{\eta_{0}\lambda_{min}}{3})^{t}R_{0}$$
(65)

where θ_t is some linear interpolation between θ_t and θ_{t+1} .

$$\begin{aligned} \left\| I - \eta J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} &= \left\| I - \eta J(\theta_0) J(\theta_0)^T + \eta J(\theta_0) J(\theta_0)^T - \eta J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} \\ &= \left\| I - \eta_0 \Theta_0 + \eta J(\theta_0) J(\theta_0)^T - \eta J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} \\ &= \left\| I - \eta_0 \Theta + \eta_0 \Theta - \eta_0 \Theta_0 + \eta J(\theta_0) J(\theta_0)^T - \eta J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} \\ &\leq \left\| I - \eta_0 \Theta \right\|_{op} + \eta_0 \left\| \Theta - \Theta_0 \right\|_{op} + \eta \left\| J(\theta_0) J(\theta_0)^T - J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} \end{aligned}$$

$$(66)$$

The assumption Θ is full-rank and $\lambda_{min} > 0$ implies

$$||I - \eta_0 \Theta||_{op} = \sigma_{max}(I - \eta_0 \Theta) = 1 - \eta_0 \sigma_{min}(\Theta) = 1 - \eta_0 \lambda_{min}$$
 (67)

Because $\hat{\Theta}_0 \to \Theta$ in probability, one can find n_2 such that

$$\eta_0 \left\| \Theta - \hat{\Theta}_0 \right\|_{op} \le \eta_0 \left\| \Theta - \hat{\Theta}_0 \right\|_F \le \frac{\eta_0 \lambda_{min}}{3} \tag{68}$$

For the third part

$$\|J(\theta_{0})J(\theta_{0})^{T} - J(\tilde{\theta}_{t})J(\theta_{t})^{T}\|_{op} = \|J(\theta_{0})J(\theta_{0})^{T} - J(\theta_{0})J(\theta_{t})^{T} + J(\theta_{0})J(\theta_{t})^{T} - J(\tilde{\theta}_{t})J(\theta_{t})^{T}\|_{op}$$

$$= \|J(\theta_{0})[J(\theta_{0})^{T} - J(\theta_{t})^{T}] + [J(\theta_{0}) - J(\tilde{\theta}_{t})]J(\theta_{t})^{T}\|_{op}$$

$$\leq \|J(\theta_{0})\|_{op} \|J(\theta_{0})^{T} - J(\theta_{t})^{T}\|_{op} + \|J(\theta_{0}) - J(\tilde{\theta}_{t})\|_{op} \|J(\theta_{t})^{T}\|_{op}$$

$$\leq \|J(\theta_{0})\|_{F} \|J(\theta_{0})^{T} - J(\theta_{t})^{T}\|_{F} + \|J(\theta_{0}) - J(\tilde{\theta}_{t})\|_{F} \|J(\theta_{t})^{T}\|_{F}$$

$$\leq K\sqrt{n}K\sqrt{n}\|\theta_{0} - \theta_{t}\|_{2} + K\sqrt{n}K\sqrt{n}\|\theta_{0} - \tilde{\theta}_{t}\|_{2}$$

$$= K^{2}n\|\theta_{t} - \theta_{0}\|_{2} + K^{2}n\|\tilde{\theta}_{t} - \theta_{0}\|_{2}$$

$$\leq 2K^{2}n\frac{3KR_{0}}{\lambda_{min}}n^{-\frac{1}{2}}$$

Take the three parts together and when $n \ge \left(\frac{18K^3R_0}{\lambda_{min}}\right)^2$,

$$\left\| 1 - \eta J(\tilde{\theta}_t) J(\theta_t)^T \right\|_{op} \le 1 - \eta_0 \lambda_{min} + \frac{\eta_0 \lambda_{min}}{3} + 2\eta_0 K^2 \frac{3KR_0}{\lambda_{min}} n^{-\frac{1}{2}}$$

$$\le 1 - \frac{\eta_0 \lambda_{min}}{3}$$
(70)

Take this into (65),

$$\|g(\theta_{t+1})\|_{2} \le (1 - \frac{\eta_{0}\lambda_{min}}{3})^{t+1}R_{0}$$
 (71)

For (57),

$$\begin{split} \left\| \hat{\Theta}_{0} - \hat{\Theta}_{t} \right\|_{F} &= \frac{1}{n} \left\| J(\theta_{0}) J(\theta_{0})^{T} - J(\theta_{t}) J(\theta_{t})^{T} \right\|_{F} \\ &= \frac{1}{n} \left\| J(\theta_{0}) J(\theta_{0})^{T} - J(\theta_{0}) J(\theta_{t})^{T} + J(\theta_{0}) J(\theta_{t})^{T} - J(\theta_{t}) J(\theta_{t})^{T} \right\|_{F} \\ &= \frac{1}{n} \left\| J(\theta_{0}) [J(\theta_{0})^{T} - J(\theta_{t})^{T}] + [J(\theta_{0}) - J(\theta_{t})] J(\theta_{t})^{T} \right\|_{F} \\ &\leq \frac{1}{n} \left\| J(\theta_{0}) \right\|_{F} \left\| J(\theta_{0})^{T} - J(\theta_{t})^{T} \right\|_{F} + \frac{1}{n} \left\| J(\theta_{0}) - J(\theta_{t}) \right\|_{F} \left\| J(\theta_{t})^{T} \right\|_{F} \\ &\leq K^{2} \left\| \theta_{t} - \theta_{0} \right\|_{2} + K^{2} \left\| \theta_{t} - \theta_{0} \right\|_{2} \\ &\leq \frac{6K^{3}R_{0}}{\lambda_{min}} n^{-\frac{1}{2}} \end{split}$$

$$(72)$$

6.2 Bounding $||f_t(x) - f_t^{lin}(x)||_2$

To simplify the notation, let $g^{lin}(t) = f_t^{lin}(\mathcal{X}) - \mathcal{Y}$ and $g(t) = f_t(\mathcal{X}) - \mathcal{Y}$.

Theorem H.1. Same as in Theorem G.2. For every $x \in \mathbb{R}^{n_0}$ with $||x||_2 \leq 1$, for $\delta_0 > 0$ arbitrarily small, there exist $R_0 > 0$ and $N \in \mathbb{N}$ such that for every $n \geq N$, with probability at least $(1 - \delta_0)$ over random initialization,

$$\sup_{t} \|g^{lin}(t) - g(t)\|_{2}, \quad \sup_{t} \|g^{lin}(t, x) - g(t, x)\|_{2} \lesssim n^{-\frac{1}{2}} R_{0}^{2}$$
(73)

Proof.

Recall

$$\dot{f}_t(\mathcal{X}) = -\eta \hat{\Theta}_t(\mathcal{X}, \mathcal{X}) \left(f_t(\mathcal{X}) - \mathcal{Y} \right) \tag{74}$$

$$\dot{f}_t^{lin}(\mathcal{X}) = -\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X}) \left(f_t^{lin}(\mathcal{X}) - \mathcal{Y} \right) \tag{75}$$

$$f_t^{lin}(\mathcal{X}) = e^{-\eta \hat{\Theta}_0(\mathcal{X}, \mathcal{X})t} (f_0(\mathcal{X}) - \mathcal{Y}) + \mathcal{Y}$$
(76)

That is

$$\dot{g}(t) = -\eta \hat{\Theta}_t g(t) \tag{77}$$

$$\dot{g}^{lin}(t) = -\eta \hat{\Theta}_0 g^{lin}(t) \tag{78}$$

$$g^{lin}(t) = e^{-\eta \hat{\Theta}_0 t} g^{lin}(0) \tag{79}$$

$$\frac{d}{dt} \left(e^{\eta \hat{\Theta}_0 t} \left(g^{lin}(t) - g(t) \right) \right)
= \frac{d}{dt} \left(g^{lin}(0) - e^{\eta \hat{\Theta}_0 t} g(t) \right)
= 0 - \eta \hat{\Theta}_0 e^{\eta \hat{\Theta}_0 t} g(t) + e^{\eta \hat{\Theta}_0 t} \eta \hat{\Theta}_t g(t)
= -\eta e^{\eta \hat{\Theta}_0 t} \hat{\Theta}_0 g(t) + \eta e^{\eta \hat{\Theta}_0 t} \hat{\Theta}_t g(t)
= \eta e^{\eta \hat{\Theta}_0 t} \left(\hat{\Theta}_t - \hat{\Theta}_0 \right) g(t)$$
(80)

where $\hat{\Theta}_0 e^{\eta \hat{\Theta}_0 t} = \hat{\Theta}_0 \sum_{k=0}^{\infty} \frac{1}{k!} (\eta \hat{\Theta}_0 t)^k = \left(\sum_{k=0}^{\infty} \frac{1}{k!} (\eta \hat{\Theta}_0 t)^k \right) \hat{\Theta}_0 = e^{\eta \hat{\Theta}_0 t} \hat{\Theta}_0$

Integrating both sides

$$e^{\eta \hat{\Theta}_0 t} \left(g^{lin}(t) - g(t) \right) = \int_0^t \eta e^{\eta \hat{\Theta}_0 s} \left(\hat{\Theta}_s - \hat{\Theta}_0 \right) g(s) \, \mathrm{d}s \tag{81}$$

$$g^{lin}(t) - g(t) = \int_0^t \eta e^{\eta \hat{\Theta}_0(s-t)} (\hat{\Theta}_s - \hat{\Theta}_0) g(s) ds$$
 (82)

This is not easy to bound, so we add a $g^{lin}(s)$ term.

$$g^{lin}(t) - g(t) = -\int_0^t \eta e^{\eta \hat{\Theta}_0(s-t)} (\hat{\Theta}_s - \hat{\Theta}_0) (g^{lin}(s) - g(s)) ds$$
$$+ \int_0^t \eta e^{\eta \hat{\Theta}_0(s-t)} (\hat{\Theta}_s - \hat{\Theta}_0) g^{lin}(s) ds$$
(83)

$$||g^{lin}(t) - g(t)||_{2} \le \eta \int_{0}^{t} ||e^{\eta \hat{\Theta}_{0}(s-t)}||_{op} ||(\hat{\Theta}_{s} - \hat{\Theta}_{0})||_{op} ||g^{lin}(s) - g(s)||_{2} ds + \eta \int_{0}^{t} ||e^{\eta \hat{\Theta}_{0}(s-t)}||_{op} ||(\hat{\Theta}_{s} - \hat{\Theta}_{0})||_{op} ||g^{lin}(s)||_{2} ds$$
(84)

where the $\|\cdot\|_{op}$ is the induced 2-norm for a matrix.

If λ is an eigenvalue of $\hat{\Theta}_0$, then e^{λ} is an eigenvalue of $e^{\hat{\Theta}_0}$. Let $\lambda_0 > 0$ be the smallest eigenvalue of $\hat{\Theta}_0$. Since s - t < 0, $\lambda_0 \eta(s - t) < 0$ is the largest eigenvalue of $\hat{\Theta}_0 \eta(s - t)$.

$$\left\| e^{\eta \hat{\Theta}_0(s-t)} \right\|_{op} = \sigma_{max}(e^{\eta \hat{\Theta}_0(s-t)}) = e^{\lambda_0 \eta(s-t)}$$
(85)

Take this into the equation,

$$||g^{lin}(t) - g(t)||_{2} \leq \eta \int_{0}^{t} e^{\lambda_{0}\eta(s-t)} ||(\hat{\Theta}_{s} - \hat{\Theta}_{0})||_{op} ||g^{lin}(s) - g(s)||_{2} ds + \eta \int_{0}^{t} e^{\lambda_{0}\eta(s-t)} ||(\hat{\Theta}_{s} - \hat{\Theta}_{0})||_{op} ||g^{lin}(s)||_{2} ds$$
(86)

$$e^{\lambda_0 \eta t} \|g^{lin}(t) - g(t)\|_{2} \leq \eta \int_{0}^{t} e^{\lambda_0 \eta s} \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} \|g^{lin}(s) - g(s)\|_{2} ds + \eta \int_{0}^{t} e^{\lambda_0 \eta s} \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} \|g^{lin}(s)\|_{2} ds$$

$$(87)$$

Let

$$u(t) \equiv e^{\lambda_0 \eta t} \left\| g^{lin}(t) - g(t) \right\|_2 \tag{88}$$

$$\alpha(t) \equiv \eta \int_0^t e^{\lambda_0 \eta s} \left\| \left(\hat{\Theta}_s - \hat{\Theta}_0 \right) \right\|_{op} \left\| g^{lin}(s) \right\|_2 ds \tag{89}$$

$$\beta(t) \equiv \eta \left\| \left(\hat{\Theta}_t - \hat{\Theta}_0 \right) \right\|_{op} \tag{90}$$

The above can be written as

$$u(t) \le \alpha(t) + \int_0^t \beta(s)u(s) \,\mathrm{d}s \tag{91}$$

Since $e^{\lambda_0 \eta s} \| (\hat{\Theta}_s - \hat{\Theta}_0) \|_{op} \| g^{lin}(s) \|_2 \ge 0$, $\alpha(t)$ is non-decreasing. Applying an integral form of the Grönwall's inequality gives

$$u(t) \le \alpha(t)e^{\int_0^t \beta(s) \, \mathrm{d}s} \tag{92}$$

Recall

$$\|g^{lin}(t)\|_{2} = \|e^{-\eta \hat{\Theta}_{0} t} g^{lin}(0)\|_{2} \le \|e^{-\eta \hat{\Theta}_{0} t}\|_{on} \|g^{lin}(0)\|_{2} = e^{-\lambda_{0} \eta t} \|g^{lin}(0)\|_{2}$$

$$(93)$$

Then

$$\alpha(t) = \eta \int_{0}^{t} e^{\lambda_{0}\eta s} \left\| (\hat{\Theta}_{s} - \hat{\Theta}_{0}) \right\|_{op} \left\| g^{lin}(s) \right\|_{2} ds$$

$$\leq \eta \int_{0}^{t} e^{\lambda_{0}\eta s} \left\| (\hat{\Theta}_{s} - \hat{\Theta}_{0}) \right\|_{op} e^{-\eta \lambda_{0} t} \left\| g^{lin}(0) \right\|_{2} ds$$

$$= \eta \left\| g^{lin}(0) \right\|_{2} \int_{0}^{t} e^{\lambda_{0}\eta(s-t)} \left\| (\hat{\Theta}_{s} - \hat{\Theta}_{0}) \right\|_{op} ds$$

$$\leq \eta \left\| g^{lin}(0) \right\|_{2} \int_{0}^{t} \left\| (\hat{\Theta}_{s} - \hat{\Theta}_{0}) \right\|_{op} ds$$

$$\leq \eta \left\| g^{lin}(0) \right\|_{2} \int_{0}^{t} \left\| (\hat{\Theta}_{s} - \hat{\Theta}_{0}) \right\|_{op} ds$$
(94)

since $e^{\lambda_0 \eta(s-t)} \le 1$.

Take this into (92),

$$e^{\lambda_{0}\eta t} \|g^{lin}(t) - g(t)\|_{2} \leq \eta \int_{0}^{t} e^{\lambda_{0}\eta s} \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} \|g^{lin}(s)\|_{2} ds e^{\int_{0}^{t} \eta \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} ds}$$

$$\leq \eta \|g^{lin}(0)\|_{2} \int_{0}^{t} \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} ds e^{\int_{0}^{t} \eta \|(\hat{\Theta}_{s} - \hat{\Theta}_{0})\|_{op} ds}$$

$$(95)$$

Let $\sigma_t = \sup_{0 \le s \le t} \left\| \left(\hat{\Theta}_s - \hat{\Theta}_0 \right) \right\|_{op}$. Then

$$e^{\lambda_0 \eta t} \|g^{lin}(t) - g(t)\|_{2} \leq \eta \|g^{lin}(0)\|_{2} \int_{0}^{t} \sigma_{t} \, \mathrm{d}s \, e^{\int_{0}^{t} \eta \sigma_{t} \, \mathrm{d}s}$$

$$= \eta \|g^{lin}(0)\|_{2} \sigma_{t} t \, e^{\sigma_{t} \eta t}$$

$$= \sigma_{t} \eta t e^{\sigma_{t} \eta t} \|g^{lin}(0)\|_{2}$$
(96)

$$\|g^{lin}(t) - g(t)\|_{2} \le \sigma_{t} \eta t e^{\sigma_{t} \eta t - \lambda_{0} \eta t} \|g^{lin}(0)\|_{2}$$
 (97)

As it is proved in Theorem G.1,

$$\sigma_t = \sup_{0 \le s \le t} \left\| \left(\hat{\Theta}_s - \hat{\Theta}_0 \right) \right\|_{op} \le \sup_t \left\| \left(\hat{\Theta}_t - \hat{\Theta}_0 \right) \right\|_F \lesssim n^{-\frac{1}{2}} R_0 \to 0 \tag{98}$$

when $n_1 = \cdots = n_L = n \to \infty$. Thus for large n,

$$\eta t e^{\eta \sigma_t t - \lambda_0 \eta t} = \frac{\eta t}{e^{\eta t (\lambda_0 - \sigma_t)}} = \mathcal{O}(1)$$
(99)

Recall $g(0) = g^{lin}(0)$ are gaussian distributed and there exist

$$||g^{lin}(0)||_2 = ||g(0)||_2 < R_0$$
 (100)

Therefore

$$\|g^{lin}(t) - g(t)\|_{2} \lesssim \sigma_{t} R_{0} \lesssim n^{-\frac{1}{2}} R_{0}^{2} \to 0$$
 (101)

as $n \to \infty$.

References

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