### **STAT 946:**

## Lecture 11: Feature Learning

October 21, 2025 • Scribed by: Edward Chang

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# 1 Feature Learning

#### 1.1 High-level points

- Non-kernel learning.
- Non-linear regime (beyond fixed NTK).

## 1.2 Recall: 1-layer network (NTK scaling)

We consider a single-hidden-layer network under NTK scaling

$$f(x;\theta) = \frac{1}{\sqrt{n}} W_1 \phi(W_0 x), \qquad x \in \mathbb{R}^{n_0}, \ W_0 \in \mathbb{R}^{n \times n_0}, \ W_1 \in \mathbb{R}^{1 \times n},$$
 (1)

with width m and elementwise nonlinearity  $\phi$ .

#### 1.3 Loss and training

Given data  $\{(x^{\alpha}, y^{\alpha})\}_{\alpha=1}^{n}$ , use the squared loss

$$L(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left( f(x^{\alpha}; \theta) - y^{\alpha} \right)^{2}. \tag{2}$$

A gradient step with constant Learning Rate  $\eta > 0$  is

$$\theta_{k+1} = \theta_k - \eta \nabla L(\theta_k). \tag{3}$$

#### 1.4 Hidden features

Write the hidden features at step k as

$$h^{\alpha}(\theta) = W_0 x^{\alpha} \in \mathbb{R}^m. \tag{4}$$

#### 1.5 Feature dynamics

For a training point  $x^n$ , define

$$\Delta h^{\alpha} := h^{(\alpha)}(\theta_1) - h^{(\alpha)}(\theta_0). \tag{5}$$

A gradient step on  $W_0$  yields a change of the form

$$\Delta h^{\alpha} = -\frac{\eta}{m\sqrt{n}} \sum_{\beta=1}^{N} \left( f^{\beta} - y^{\beta} \right) \langle x^{\alpha}, x^{\beta} \rangle W_{1}^{\top} \otimes \phi'(h^{\beta}), \tag{6}$$

We note that as  $n \to \infty$ ,

$$\eta, m, f^{\beta}, y^{\beta}, x^{\alpha}, x^{\beta}, W_1, \phi'(h^{\beta}) = \mathcal{O}(1)$$

hence,

$$\Delta h^{\alpha} = \mathcal{O}\left(\frac{1}{\sqrt{n}}\right) \tag{7}$$

Now, consider back to NTK. The (discrete) flow can be written with the NTK:

$$\Delta f^{\alpha} = \frac{\eta}{m} K^{(\alpha)}(f - y) = \mathcal{O}(1) \tag{8}$$

But we need  $\Delta h^{\alpha} = \mathcal{O}(1)$  instead of  $\mathcal{O}(n^{-1/2})$  for NTK to evolve.

# 2 Scaling Tweaks

### 2.1 Naive modification

Set the learning rate to

$$\eta = \eta_0 \sqrt{n}$$
.

Then

$$\Delta h^{\alpha} = \mathcal{O}(1), \qquad \Delta f^{\alpha} = \mathcal{O}(\sqrt{n}) \text{ (diverges)}.$$

Remark: for cross-entropy loss this can still work (as noted in class).

#### 2.2 Compromise: scale down the output

Use

$$f(x,\theta) = \frac{1}{n} W_1 \phi(W_0 x). \tag{9}$$

Under this scaling,

$$\Delta h^k = \mathcal{O}\left(\frac{1}{\sqrt{n}}\right), \qquad \Delta f^k = \mathcal{O}\left(\frac{1}{\sqrt{n}}\right),$$

so changes are controlled (cf. the original where  $\Delta h^k = \mathcal{O}(1)$  but  $\Delta f^k = \mathcal{O}(\sqrt{n})$ ).

#### 2.3 Mean-field parameterization

Pre-factor is 1/n; choose the learning rate

$$\eta = \eta_0 n$$

which accelerates the hidden layer and escapes the strict kernel regime:

$$\Delta h^k = \mathcal{O}(1), \qquad \Delta f^k = \mathcal{O}(1).$$

#### 2.4 Comparison

|            | Prefactor        | $\mathbf{L}\mathbf{R}$ | Init sd          |
|------------|------------------|------------------------|------------------|
| NTK (W1)   | $1/\sqrt{n}$ (1) | $1 (1/\sqrt{n})$       | $1 (1/\sqrt{n})$ |
| Mean field | 1/n              | n                      | 1                |

In bracket is what people use in practice.

#### Remarks

- "ABC reparameterization"
- NTK linearized dynamics:

$$\Delta f \approx -\frac{\eta}{n} K(f-y),$$

which stays kernel-like unless features move. In the mean-field scaling, the *state space* dynamics are genuinely parameter-driven (nonlinear) rather than purely kernel.

• Full-parameter update:  $\theta_{k+1} = \theta_k - \eta \nabla L(\theta_k)$ , vs. NTK linearized in function space f (with neurons summarized via h, g [(placeholders to match board notation)]).

#### 3 Mean-Field ODE

#### 3.1 Network as an integral against an empirical measure

$$f(x;\theta) = \frac{1}{n} \sum_{i=1}^{n} w_{1,i} \, \phi(\langle w_{0,i}, x \rangle) = \int u(\langle w, x \rangle) \, d\rho^{(n)}(w, u), \tag{10}$$

where the *empirical measure* on parameter space is

$$\rho^{(n)} = \frac{1}{n} \sum_{i=1}^{n} \delta_{(w_{0,i}, w_{1,i})}.$$

#### 3.2 Gradient flow (finite width)

Denote the population risk  $L(\theta)$ . Gradient flow is

$$\frac{d}{dt}\theta(t) = \partial_t \theta(t) = -\eta \nabla L(\theta(t)).$$

At the particle level, this induces ODEs for each  $(w_{0,i}, w_{1,i})$  (indices suppressed for clarity):

$$\partial_t w_{1,i} = -\frac{1}{m} \sum_{\beta=1}^n \left( f^{\beta}(t) - y^{\beta} \right) \phi \left( \langle w_{0,i}, x^{\beta} \rangle \right),$$

$$\partial_t w_{0,i} = -\frac{1}{m} \sum_{\beta=1}^n \left( f^{\beta}(t) - y^{\beta} \right) W_1 \, \phi' \left( \langle w_{0,i}, x^{\beta} \rangle \right) x^{\beta}.$$

Equivalently, the empirical measure  $\rho_t^{(n)}$  evolves by transporting each particle according to a vector field

$$\partial_t \theta_i(t) = b(\theta_i(t), \rho_t^{(n)}),$$

this is called mean-field ODE (McKean-Vlason).

### 3.3 Propagation of chaos

As  $n \to \infty$ ,

$$\rho_t^{(n)} \implies \rho_t, \qquad \mathcal{L}(\theta_i(t)) \implies \rho_t,$$

where  $\rho_t$  mean field measure,  $\rho_t^{(n)}$  all particles,  $L(\theta_i(t))$  contains one particle. This is quite surprising.

Stronger Notation:

for each fixed  $k: \mathcal{L}(\theta_1(t), \dots, \theta_k(t)) \implies \rho_t^{\otimes k}$  (asymptotic k-particle independence).

A quantitative bound (for a suitable metric, e.g. Wasserstein-2) takes the form

$$W_2\Big(\mathcal{L}\big(\theta_1(t),\ldots,\theta_k(t)\big),\,\rho_t^{\otimes k}\Big) \lesssim \frac{1}{n}e^{c(t,n_0)}.$$

#### 4 Mean-Field PDE

#### 4.1 Test functions and weak derivatives

- 1. We generally cannot differentiate  $\rho_t^{(n)}, \delta_{\theta}(t)$ .
- 2. The standard trick is to use a test function  $q \in C_c^{\infty}(\mathbb{R}^{n_0+1})$  (smooth with compact support).

Informally, let's pretend the following works. (weak derivative)

$$\int q(\theta) \nabla_{\theta} \rho_t^{(n)}(\theta) d\theta \stackrel{IBP}{=} - \int \nabla_{\theta} q(\theta) d\rho_t^{(n)}(\theta)$$

Now consider,

$$\partial_t \int q(\theta) \, \rho_t^{(n)}(d\theta) = \frac{1}{n} \sum_{i=1}^n \langle \nabla_\theta q(\theta_i(t)), \, \partial_t \theta_i(t) \rangle = \int \langle \nabla_\theta q(\theta), \, b(\theta, \, \rho_t^{(n)}) \rangle \, \rho_t^{(n)}(d\theta).$$

$$= \int \nabla_\theta q(\theta) b(\theta, \, \rho_t^{(n)}) d\rho_t^{(n)}$$

Further, imagine this works:

$$\int \langle \nabla_{\theta} q(\theta), b(\theta \mid \rho_t^{(n)}) \rangle \, \rho_t^{(n)}(d\theta) \stackrel{IBP}{=} \int q(\theta) \left[ -\operatorname{div}_{\theta} \left( b(\theta \mid \rho_t^{(n)}) \, \rho_t^{(n)}(\theta) \right) \right] d\theta$$
$$= \int q(\theta) \partial_t \rho_t^{(n)}(\theta) d\theta$$

And this is valid for any q. Hence  $\rho_t^{(n)}$  is a weak solution of the continuity/transport PDE. We define the first order non-linear "Transport Equation":

$$\partial_t \rho_t = -\operatorname{div} \left( b(\theta, \rho_t) \rho_t \right),$$

$$\rho_0 = \rho_0^{(n)}.$$
(11)

This is a first-order, nonlinear transport equation (the mean-field PDE).

# References:

- 1. Mei, Montanari, & Nguyen (2018).
- 2. Chizat & Bach (2018).
- 3. Nitanda & Suzuki (2017).
- 4. Rotskoff, Vanden-Eijnden (2018).
- 5. Sirignano & Spiliopoulos (2018).