Student-T Process Instead of Gaussian Process for NTK

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Motivation

According to the paper **"Deep learning versus kernel learning: an empirical study of loss landscape geometry and the time evolution of the Neural Tangent Kernel"** (presented by 袁哥), infinite-width NTK gives a **poor prediction** on the loss of the **finite-width neural network during training** and, **final basin** chosen by a child highly **sensitive to SGD noise** and the NTK **involves very rapidly**.

Why not just add some random noise to the NTK, to simulate the unstable NTK?

With **inverse Wishart distribution** $\Sigma \sim \mathcal{IW}(\nu, K)$ where the degree of freedom $\nu > 2$ and K is positive definite, we can generate a random matrix Σ with expectation $\mathbb{E}[\Sigma] = \frac{K}{\nu-2}$.

Inverse Normal-Wishart Distribution

Consider the **randomness of the kernel matrix**, with Bayesian rule, we can model the kernel matrix with **Inverse Wishart distribution**.

$$p(y|\phi, \nu, K) = \int p(y|\phi, \Sigma)p(\Sigma|\nu, K)d\Sigma = \mathcal{TP}(\phi, K, \nu)$$

Denote Inverse Wishart distribution as $\Sigma|\nu, K \sim \mathcal{IW}(\nu, K) = p(\Sigma|\nu, K)$ and the Gaussian process as $y|\phi, \Sigma \sim \mathcal{GP}(\phi, \Sigma) = p(y|\phi, \Sigma)$. Note that the random matrix $\Sigma \in \mathbb{R}^{N \times N}$ is generated by Inverse Wishart. The hyperparameters are $K \in \mathbb{R}^{N \times N}$, $\nu \in \mathbb{R}$, $\phi \in \mathbb{R}^N$.

Finally, $\mathcal{TP}(\phi, K, \nu)$ is the **Student-T process**.

Student-T Process

The Student-T process can be written as

$$y \sim \mathcal{TP}(\phi, K, \nu)$$

The hyperparameter ν is called **degrees of freedom**, it can control the covariance of the output $cov(y) = \frac{\nu}{\nu-2}K$. Thus, the relation between $\mathcal{TP}$ and $\mathcal{GP}$ is

$$\mathcal{GP}(\phi, K) = \lim_{\nu \to \infty} \mathcal{TP}(\phi, K, \nu)$$

Student-T Process

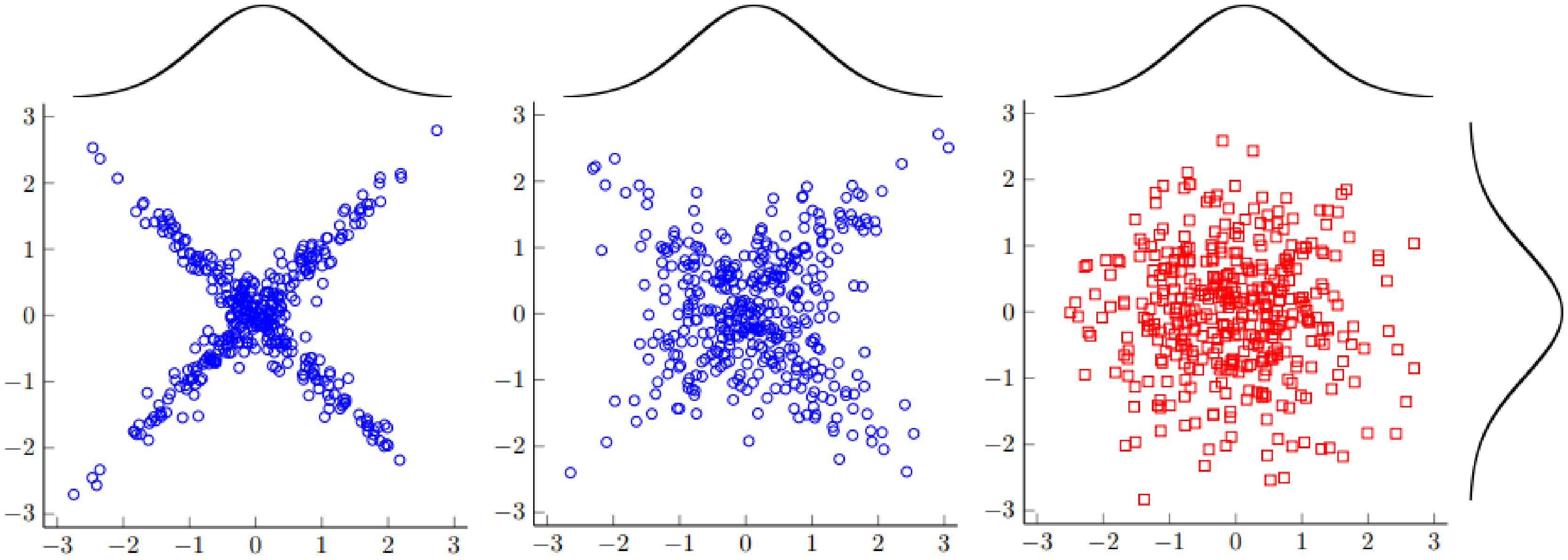


Figure 2: Uncorrelated bivariate samples from a Student-t copula with $\nu = 3$ (left), a Student-t copula with $\nu = 10$ (centre) and a Gaussian copula (right). All marginal distributions are N(0, 1) distributed.

Degrees of freedom is the number of values in the final calculation of a statistic that are free to vary.

Student-T Process Posterior

Given a training dataset $\{X_1, Y_1\}$ with n_1 samples and a testing dataset $\{X_2, Y_2\}$ with n_2 samples where $\boldsymbol{X_1} \in \mathbb{R}^{n_1 \times d}$, $\boldsymbol{Y_1} \in \mathbb{R}^{n_1}$, and $\boldsymbol{X_2} \in \mathbb{R}^{n_2 \times d}$, $\boldsymbol{Y_2} \in \mathbb{R}^{n_2}$.

Denote the mean function as z and the kernel function as k. Thus, $\phi_i = z(X_i)$ and $K_{ij} = k(X_i, X_j)$

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim \mathcal{TP}(\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix})$$

Student-T Process Posterior

The posterior is

$$y_2|y_1 \sim \mathcal{TP}(\hat{\phi}, \frac{\nu+\beta+-2}{\nu+n_1-2}\hat{K}_{22}, \nu+n_1)$$

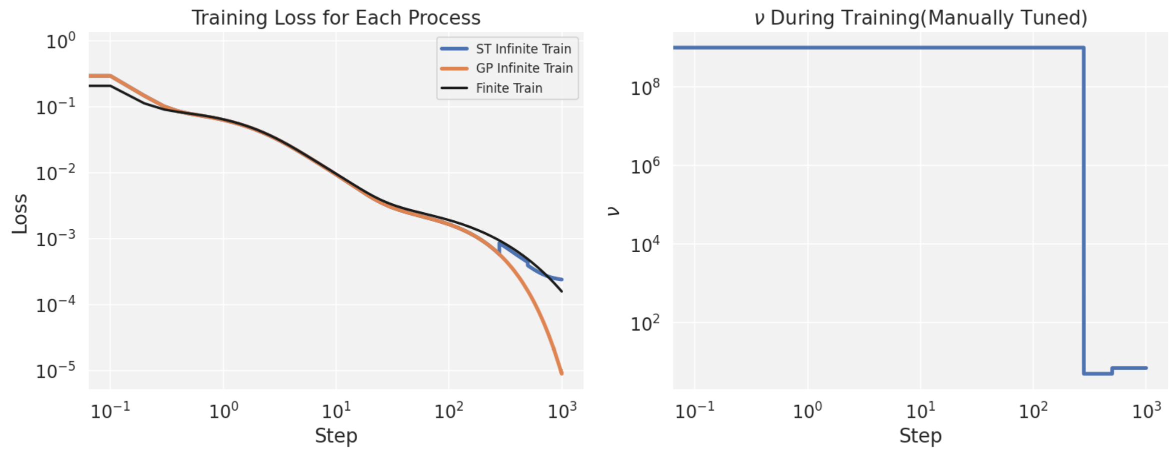
Where

$$\hat{\phi} = K_{21}K_{11}^{-1}(Y_1-\phi_1)+\phi_2$$

$$\beta = (Y_1-\phi_1)^\top K_{11}^{-1}(Y_1-\phi_1)$$

$$\hat{K}_{22} = K_{22}-K_{21}K_{11}^{-1}K_{12}$$

Experiment



We've already known, if $\nu = \infty$, the student-T process will converge to Gaussian process. In the above figure, we compare the result of **fitting a $\sin()$ function with $\mathcal{TP}$ (blue) and $\mathcal{GP}$(yellow) respectively**. The **left** part of above figure shows the **training/testing progress of fitting**. The right part is the value of ν during training progress.

As the **blue line** shows above(left part), as the **training progress goes**, **the ν gets lower**. It shows that we can **control ν of $\mathcal{TP}$ to achieve a better fitting(closer to black line, real NN training)**.

Conclusion

- During **training progress**, the ν **gets lower**.
- By controlling the value of ν of $\mathcal{TP}$, we can get a **more accurate prediction on the training loss** rather than $\mathcal{GP}$
- If the NTK follows the $\mathcal{TP}$, the **bigger training dataset**, the **larger degree of freedom of the posterior**.