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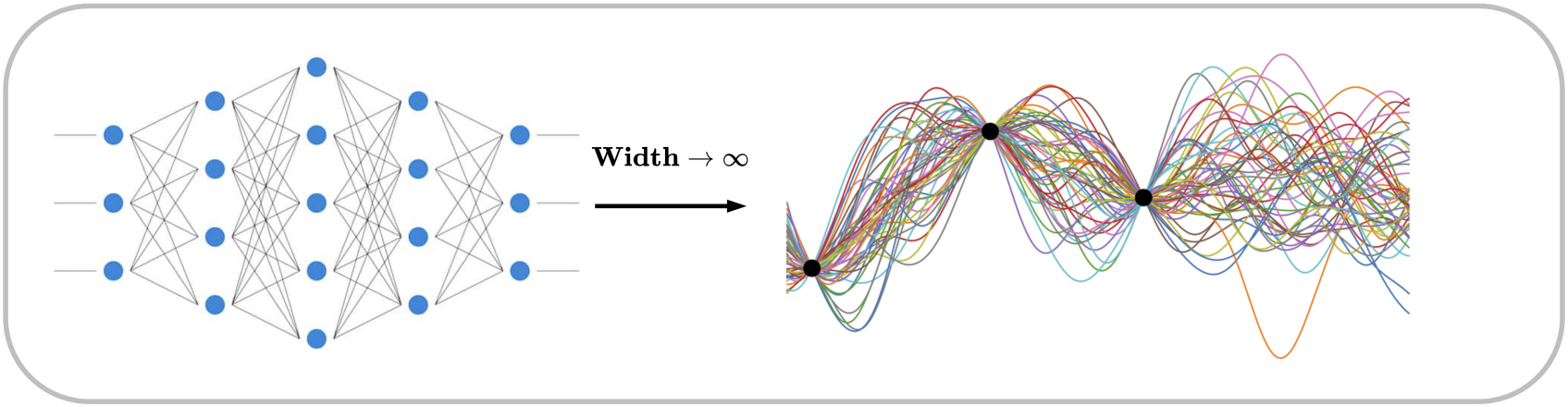
- **Virtual** meetings via Zoom (unless of course everyone is back at the lab) and hence slide presentations

Deep Neural Networks as Gaussian Processes



Jaehoon Lee, Yasaman Bahri, Roman Novak, Samuel S. Schoenholz, Jeffrey Pennington, Jascha Sohl-Dickstein

Recap: Gaussian Process

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Definition: A **Gaussian process** $\{X_t\}_{t=0}^{\infty} \sim \mathcal{GP}(0, \Sigma)$ is a stochastic process such that for any finite collection $(t_1, \ldots, t_n) \in \mathbb{R}_+^n$, we have $(X_{t_1}, \ldots, X_{t_n}) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ where $\mathbf{\Sigma}_{ij} = \Sigma(X_{t_i}, X_{t_j})$ and $\Sigma : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$

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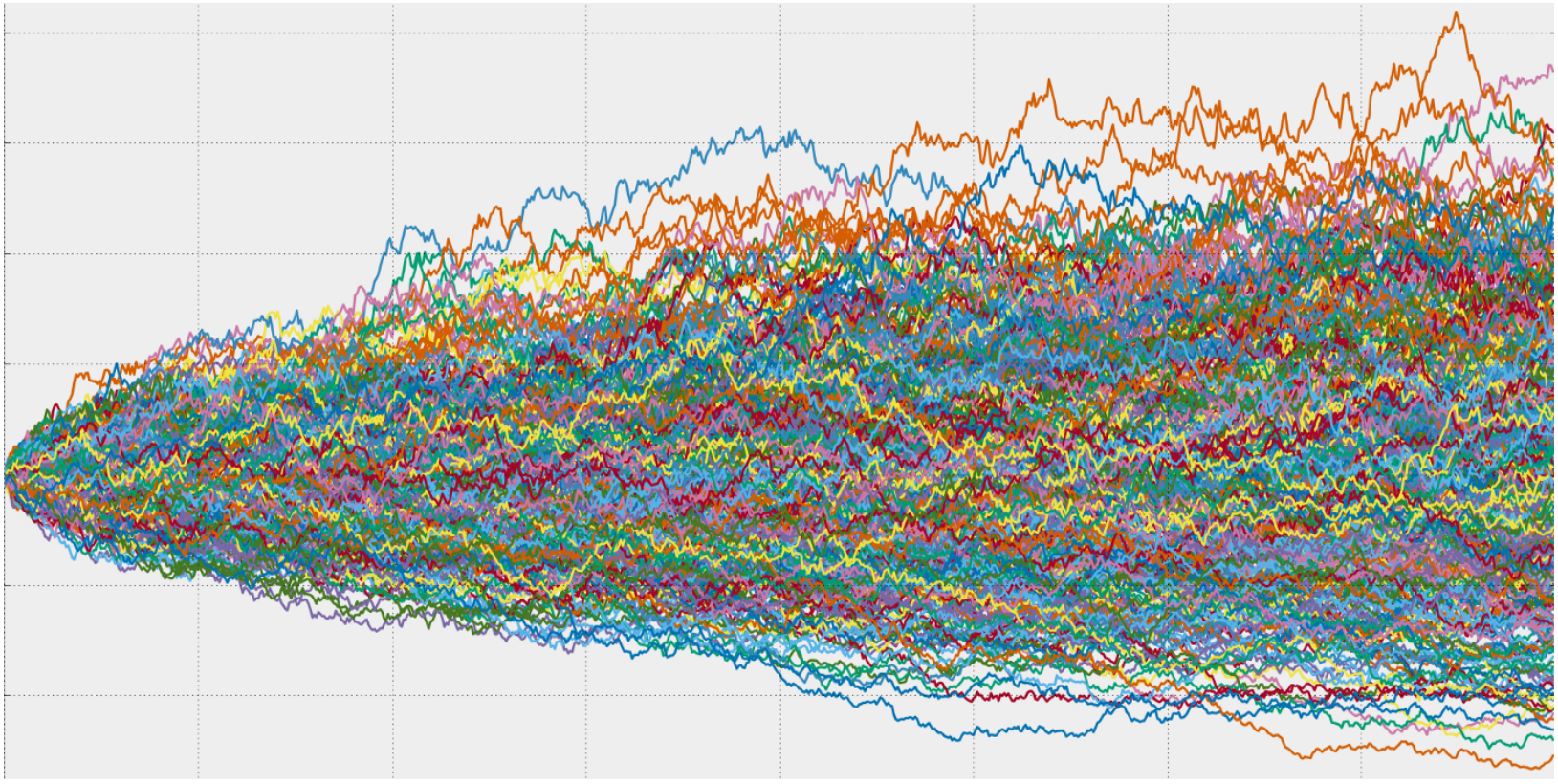
- **Example:** Brownian motion with $\Sigma(s, t) = \min(s, t)$

Sample Paths of Brownian Motion



Gaussian Processes in ML (I)

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- **Regression Problem:** Observations $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \subset \mathbb{R}^d$ and a noisy model $y_i = f(\boldsymbol{x}_i) + \epsilon_i$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$

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- Use information in the features $\boldsymbol{x}_i$ by taking approach

$$\Sigma_{ij} = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

  where $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a **symmetric** and **positive semi-definite** kernel

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- **Fact**: For $\begin{pmatrix} \boldsymbol{z}_A \\ \boldsymbol{z}_B \end{pmatrix} \sim \mathcal{N}\left(\boldsymbol{0}, \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix}\right)$ we have

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- We hence have $y^*|(\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}^*) \sim \mathcal{N}(\mu^*, \sigma^*)$ where

1 $\mu^* = K(\boldsymbol{x}^*, \boldsymbol{X}))^T \left(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 \mathbb{1}\right)^{-1} \boldsymbol{y}$

2 $\sigma^* = K(\boldsymbol{x}^*, \boldsymbol{x}^*) - K(\boldsymbol{x}^*, \boldsymbol{X})^T \left(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 \mathbb{1}\right)^{-1} K(\boldsymbol{x}^*, \boldsymbol{X})$

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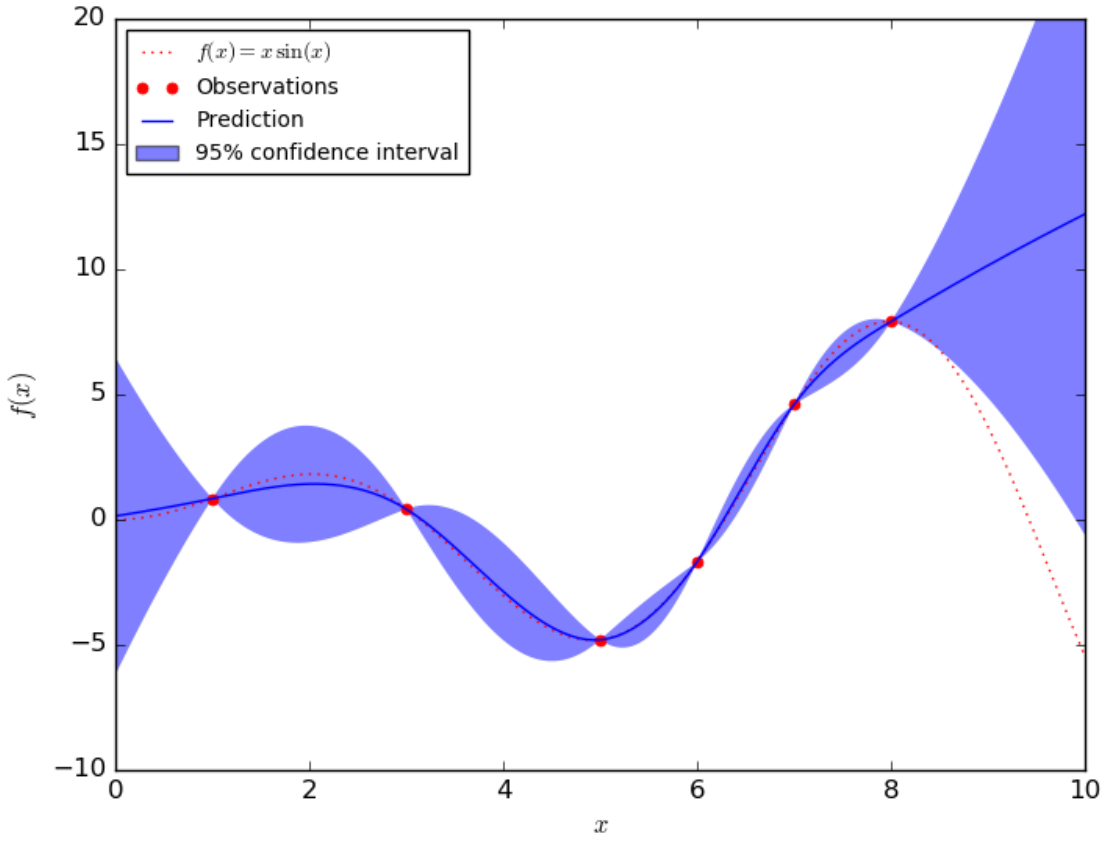

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- $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \tilde{\alpha}^{(L)}(\boldsymbol{x}) \in \mathbb{R}^{d_L}$ is the **output** of the network

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- **Effectively:** $W_{ij}^{(l)} \overset{i.i.d.}{\sim} \mathcal{N}(0, \frac{1}{d_l})$ and $b_i^{(l)} \overset{i.i.d.}{\sim} \mathcal{N}(0, \beta^2)$

  $\implies$ Usual Lecun initialization

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Theorem: *For* $\boldsymbol{X}_1 = \begin{pmatrix} X_{11} \\ \vdots \\ X_{1d} \end{pmatrix}, \ldots, \boldsymbol{X}_n = \begin{pmatrix} X_{n1} \\ \vdots \\ X_{nd} \end{pmatrix}$ *i.i.d. multi-dim. random variables with* $\mathbb{E}[\boldsymbol{X}_i] = \mathbf{0}$ *and* $cov(\boldsymbol{X}_i) = \boldsymbol{\Sigma}$*, it holds that in the limit*

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \boldsymbol{X}_i \xrightarrow{(d)} \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$$

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i.i.d. in i, where $\Sigma^{(L)}$ has the recursive structure

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for $\tilde{\boldsymbol{\Sigma}}^{(l-1)} = \begin{pmatrix} \Sigma^{(l-1)}(\boldsymbol{x}, \boldsymbol{x}) & \Sigma^{(l-1)}(\boldsymbol{x}, \boldsymbol{x'}) \\ \Sigma^{(l-1)}(\boldsymbol{x'}, \boldsymbol{x}) & \Sigma^{(l-1)}(\boldsymbol{x'}, \boldsymbol{x'}) \end{pmatrix}$

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- Allows to perform full **Bayesian-inference** with an infinitely wide neural network (no Monte Carlo methods)
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- Theory would actually break down since weights become **correlated** after just one step of SGD

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- Write limits as $f_{\boldsymbol{\theta}}^{\infty}$ and $\tilde{\alpha}_{i,\infty}^{(l)}$

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$$\begin{aligned} f_{\boldsymbol{\theta},i}(\boldsymbol{x}) &= \frac{1}{\sqrt{d_0}} \overbrace{\sum_{j=1}^{d_0} W_{ij}^{(0)} x_j} + \beta b_i^{(0)} \\ &\sim \mathcal{N}\left(0, \frac{1}{d_0} \sum_{j=1}^{d_0} \mathrm{Var}\left(W_{ij}^{(0)}\right) x_j^2 + \beta^2 \,\mathrm{Var}(b_i^{(0)})\right) \\ &\overset{(d)}{=} \mathcal{N}\left(0, \frac{1}{d_0} ||\boldsymbol{x}||_2^2 + \beta^2\right) \end{aligned}$$

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$$= \mathbb{E}\Big[\left(\frac{1}{\sqrt{d_0}} \sum_{j=1}^{d_0} W_{ij}^{(0)} x_j + \beta b_i^{(0)} \right) \left(\frac{1}{\sqrt{d_0}} \sum_{j=1}^{d_0} W_{ij}^{(0)} x'_j + \beta b_i^{(0)} \right)$$

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For any $\boldsymbol{x}, \boldsymbol{x'} \in \mathbb{R}^{d_0}$ we have:

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- **All in all:** $f_{\boldsymbol{\theta},i} \sim \mathcal{GP}(0, \Sigma^{(1)})$

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where $\tilde{\boldsymbol{\Sigma}}^{(l)} = \begin{pmatrix} \Sigma^{(l)}(\boldsymbol{x}, \boldsymbol{x}) & \Sigma^{(l)}(\boldsymbol{x}, \boldsymbol{x}') \\ \Sigma^{(l)}(\boldsymbol{x}', \boldsymbol{x}) & \Sigma^{(l)}(\boldsymbol{x}', \boldsymbol{x}') \end{pmatrix}$

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- This **concludes** the proof.

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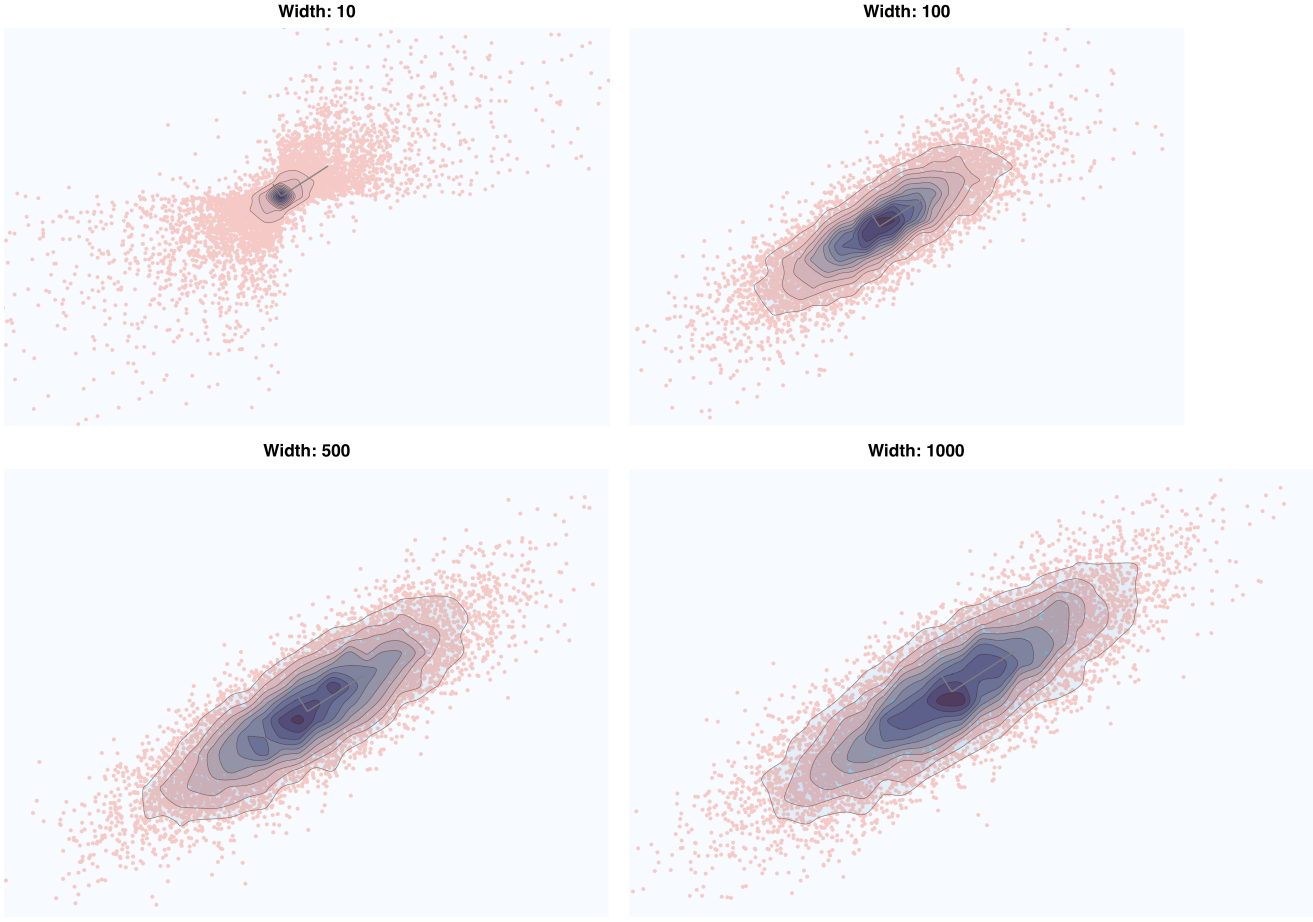

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- Can we describe $f_{\boldsymbol{\theta}}^{\infty}(\cdot)$ during **training**?

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- Even if we know how correlation evolves, CLT with correlated variables are hard to apply
- Infinite-width limit interesting because generalization gets better with **increasing width** (empirically)