Fast Finite Width (Neural) Tangent Kernel (NTK)

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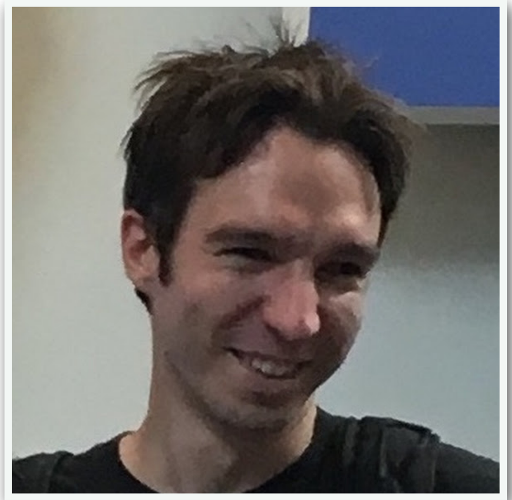
ICML 2022

$$\frac{\partial f(\theta, x_1)}{\partial \theta} \frac{\partial f(\theta, x_2)}{\partial \theta}^T$$



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June 2022

Presentation by Roman Novak

[github.com/google/neural-tangents](#)

Plan

1. **NTK definition and notation**
2. Recap of Automatic Differentiation (AD)
3. Baseline NTK computation complexity
4. Two new algorithms for computing the NTK
5. Benchmarks

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Definition

Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

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Definition

Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

The NTK is the outer product of Jacobians:

$$\Theta_\theta(x_1, x_2) := \frac{\partial f(\theta, x_1)}{\partial \theta} \frac{\partial f(\theta, x_2)}{\partial \theta}^T$$

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Definition

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Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

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$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{O}\times\mathbf{O}} := \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{O}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{O}}$$

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Definition

Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size $\mathbf{N}$

The NTK is the outer product of Jacobians:

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

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Definition

Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size $\mathbf{N}$

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$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO} \times \mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO} \times \mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P} \times \mathbf{NO}}$$

Applications in approximate inference, deep learning theory, NAS, MAML, etc.

Definition

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Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$ Batch size $\mathbf{N}$

The NTK is the outer product of Jacobians:

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

Very costly contraction: $\mathbf{N}^2\mathbf{O}^2\mathbf{P}$ time!

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Definition

Neural network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$ Batch size $\mathbf{N}$

The NTK is the outer product of Jacobians:

1000^2 for ImageNet

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

Tens of millions

Very costly contraction: $\mathbf{N}^2\mathbf{O}^2\mathbf{P}$ time!

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Definition

Neural network $f\left(\theta, x\right) \in \mathbb{R}^{\mathbf{O}}$ Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$ Batch size $\mathbf{N}$

The NTK is the outer product of Jacobians:

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

This work: reducing the contraction cost.

Very costly contraction: ~~$\mathbf{N}^2\mathbf{O}^2\mathbf{P}$~~ time!

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Recap of Automatic Differentiation (AD)

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Two fundamental AD building blocks:

- **Jacobian-vector product** $\mathrm{JVP}_{(f,\theta,x)} : \theta_t \in \mathbb{R}^{\mathbf{P}} \mapsto \frac{\partial f(\theta, x)}{\partial \theta} \theta_t \in \mathbb{R}^{\mathbf{O}}$

- **vector-Jacobian product** $\mathrm{VJP}_{(f,\theta,x)} : f_c \in \mathbb{R}^{\mathbf{O}} \mapsto \frac{\partial f(\theta, x)}{\partial \theta}^T f_c \in \mathbb{R}^{\mathbf{P}}$

Neural Network	Output size	Parameters	Batch size
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$

Recap of Automatic Differentiation (AD)

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Every other AD operation is implemented with them:

- Gradient $\texttt{grad}(f)(\theta, x) = \texttt{VJP}_{f,\theta,x}(1)$
- Reverse-mode Jacobian $\texttt{jacrev}(f)(\theta, x) = \texttt{vmap}(\texttt{VJP}_{f,\theta,x})(I_{\mathbf{O}})$
- Forward-mode Jacobian $\texttt{jacfwd}(f)(\theta, x) = \texttt{vmap}(\texttt{JVP}_{f,\theta,x})(I_{\mathbf{P}})$
- Hessian $\texttt{hessian}(f)(\theta, x) = \texttt{jacfwd}(\texttt{jacrev}(f)(\theta, x))(\theta, x)$
- ...

Neural Network	Output size	Parameters	Batch size
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$

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Recap of Automatic Differentiation (AD)

- **Time complexities of the forward pass (FP), JVP and VJP:**

Op	**Forward Pass (FP)**	**Jacobian-vector Product (JVP)**	**Vector-Jacobian Product (VJP)**
Time	$\mathbf{N}\,[\mathbf{FP}]$		

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Output size $\mathbf{O}$

Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size $\mathbf{N}$

Forward pass $[\mathbf{FP}]$

Recap of Automatic Differentiation (AD)

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- **Time complexities of the reverse-mode Jacobian:**

$$\underbrace{\frac{\partial f(\theta, x)^T}{\partial \theta}}_{\mathbf{P} \times \mathbf{O}} := \frac{\partial f(\theta, x)}{\partial \theta}^T I_{\mathbf{O}} = \underbrace{\left[\mathrm{VJP}_{(f,\theta,x)}\left(e_1\right), \ldots, \mathrm{VJP}_{(f,\theta,x)}\left(e_{\mathbf{O}}\right)\right]}_{\mathbf{O}\ \mathrm{VJPs}}$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Recap of Automatic Differentiation (AD)

Given Jacobian definitions, we can compute its cost via JVP/VJP costs.

Op	Forward Pass (FP)	Jacobian-vector Product (JVP)	Vector-Jacobian Product (VJP)	Jacobian (reverse-mode)
Time	$\mathbf{N}\,[\mathbf{FP}]$			$\mathbf{N}\mathbf{O}\,[\mathbf{FP}]$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Output size $\mathbf{O}$

Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size $\mathbf{N}$

Forward pass $[\mathbf{FP}]$

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Baseline: Jacobian contraction

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Recall that we want to compute

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

Baseline: Jacobian contraction

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Baseline algorithm: compute two Jacobians and contract them.

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

Reverse-mode Jacobian + contraction

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Baseline: Jacobian contraction

Baseline algorithm: compute two Jacobians and contract them.

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO} \times \mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO} \times \mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P} \times \mathbf{NO}}$$

Reverse-mode Jacobian + $\mathbf{N}^2\mathbf{O}^2\mathbf{P}$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Baseline: Jacobian contraction

Baseline algorithm: compute two Jacobians and contract them.

$$\underbrace{\Theta_\theta(x_1, x_2)}_{\mathbf{NO}\times\mathbf{NO}} = \underbrace{\frac{\partial f(\theta, x_1)}{\partial \theta}}_{\mathbf{NO}\times\mathbf{P}} \underbrace{\frac{\partial f(\theta, x_2)}{\partial \theta}^T}_{\mathbf{P}\times\mathbf{NO}}$$

$$\mathbf{NO}\,[\mathbf{FP}] + \mathbf{NO}\,[\mathbf{FP}] + \mathbf{N}^2\mathbf{O}^2\mathbf{P}$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

Baseline: Jacobian contraction

Method	Jacobian Contraction
Time	$\mathbf{N}\mathbf{O}\,[\mathbf{FP}] + \mathbf{N}^2\mathbf{O}^2\mathbf{P}$

Neural Network

$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Output size

$\mathbf{O}$

Parameters

$\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size

$\mathbf{N}$

Forward pass

$[\mathbf{FP}]$

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Idea 1: NTK-vector products

Similarly to Jacobians, compute the NTK via NTK-vector products applied to $\mathbf{O}$ columns of the identity matrix $I_{\mathbf{O}}$.

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Idea 1: NTK-vector products

Similarly to Jacobians, compute the NTK via NTK-vector products applied to $\mathbf{O}$ columns of the identity matrix $I_{\mathbf{O}}$. For $\mathbf{N} = 1$:

Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

For a single input column v:

$$\Theta_\theta(x_1, x_2)v$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

For a single input column v:

$$\Theta_\theta(x_1, x_2) v = \frac{\partial f(\theta, x_1)}{\partial \theta} \frac{\partial f(\theta, x_2)}{\partial \theta}^T v$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

For a single input column v:

$$\Theta_\theta(x_1, x_2)v = \frac{\partial f\left(\theta, x_1\right)}{\partial \theta} \frac{\partial f\left(\theta, x_2\right)}{\partial \theta}^T v = \frac{\partial f\left(\theta, x_1\right)}{\partial \theta} \mathrm{VJP}_{(f, \theta, x_2)}\left(v\right)$$

Neural Network $f\left(\theta, x\right) \in \mathbb{R}^{\mathbf{O}}$

Output size $\mathbf{O}$

Parameters $\theta \in \mathbb{R}^{\mathbf{P}}$

Batch size $\mathbf{N}$

Forward pass $[\mathbf{FP}]$

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Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

For a single input column v:

$$\Theta_\theta(x_1, x_2)v = \frac{\partial f(\theta, x_1)}{\partial \theta} \frac{\partial f(\theta, x_2)}{\partial \theta}^T v = \frac{\partial f(\theta, x_1)}{\partial \theta} \mathrm{VJP}_{(f,\theta,x_2)}(v) = \mathrm{JVP}_{(f,\theta,x_1)}\left[\mathrm{VJP}_{(f,\theta,x_2)}(v)\right]$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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For a single input column v:

$[\mathbf{FP}]$

$$\Theta_\theta(x_1, x_2)v = \frac{\partial f(\theta, x_1)}{\partial \theta}\frac{\partial f(\theta, x_2)}{\partial \theta}^T v = \frac{\partial f(\theta, x_1)}{\partial \theta}\mathrm{VJP}_{(f,\theta,x_2)}(v) = \boxed{\mathrm{JVP}_{(f,\theta,x_1)}\left[\mathrm{VJP}_{(f,\theta,x_2)}(v)\right]}$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Similarly to Jacobians, compute the NTK via NTK-vector products applied to $\mathbf{O}$ columns of the identity matrix $I_{\mathbf{O}}$. For $\mathbf{N} = 1$:

Evaluate $\Theta_\theta(x_1, x_2) = \Theta_\theta(x_1, x_2) I_{\mathbf{O}}$ row-by-row.

(repeat $\mathbf{O}$ times)

$\mathbf{O}\,[\mathbf{FP}]$

For a single input column v:

$$\Theta_\theta(x_1, x_2)v = \frac{\partial f(\theta, x_1)}{\partial \theta}\frac{\partial f(\theta, x_2)}{\partial \theta}^T v = \frac{\partial f(\theta, x_1)}{\partial \theta}\mathrm{VJP}_{(f,\theta,x_2)}(v) = \mathrm{JVP}_{(f,\theta,x_1)}\left[\mathrm{VJP}_{(f,\theta,x_2)}(v)\right]$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Idea 1: NTK-vector products

Batched setting: needs to be done for every pair of x_1 and x_2!

$$\mathbf{N}^2\mathbf{O}\,[\mathbf{FP}]$$

$$\Theta_\theta(x_1, x_2)v = \frac{\partial f(\theta, x_1)}{\partial \theta}\frac{\partial f(\theta, x_2)}{\partial \theta}^T v = \frac{\partial f(\theta, x_1)}{\partial \theta}\mathrm{VJP}_{(f,\theta,x_2)}(v) = \mathrm{JVP}_{(f,\theta,x_1)}\left[\mathrm{VJP}_{(f,\theta,x_2)}(v)\right]$$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

Idea 1: NTK-vector products

Method	Jacobian Contraction	NTK-vector products
Time	$\mathbf{N}\mathbf{O}\,[\mathbf{FP}] + \mathbf{N}^2\mathbf{O}^2\mathbf{P}$	$\mathbf{N}^2\mathbf{O}\,[\mathbf{FP}]$

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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Idea 2: Structured derivatives

Exploit the structure in primitive derivatives for computing the NTK.

Neural Network	Output size	Parameters	Batch size	Forward pass
$f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$	$\mathbf{O}$	$\theta \in \mathbb{R}^{\mathbf{P}}$	$\mathbf{N}$	$[\mathbf{FP}]$

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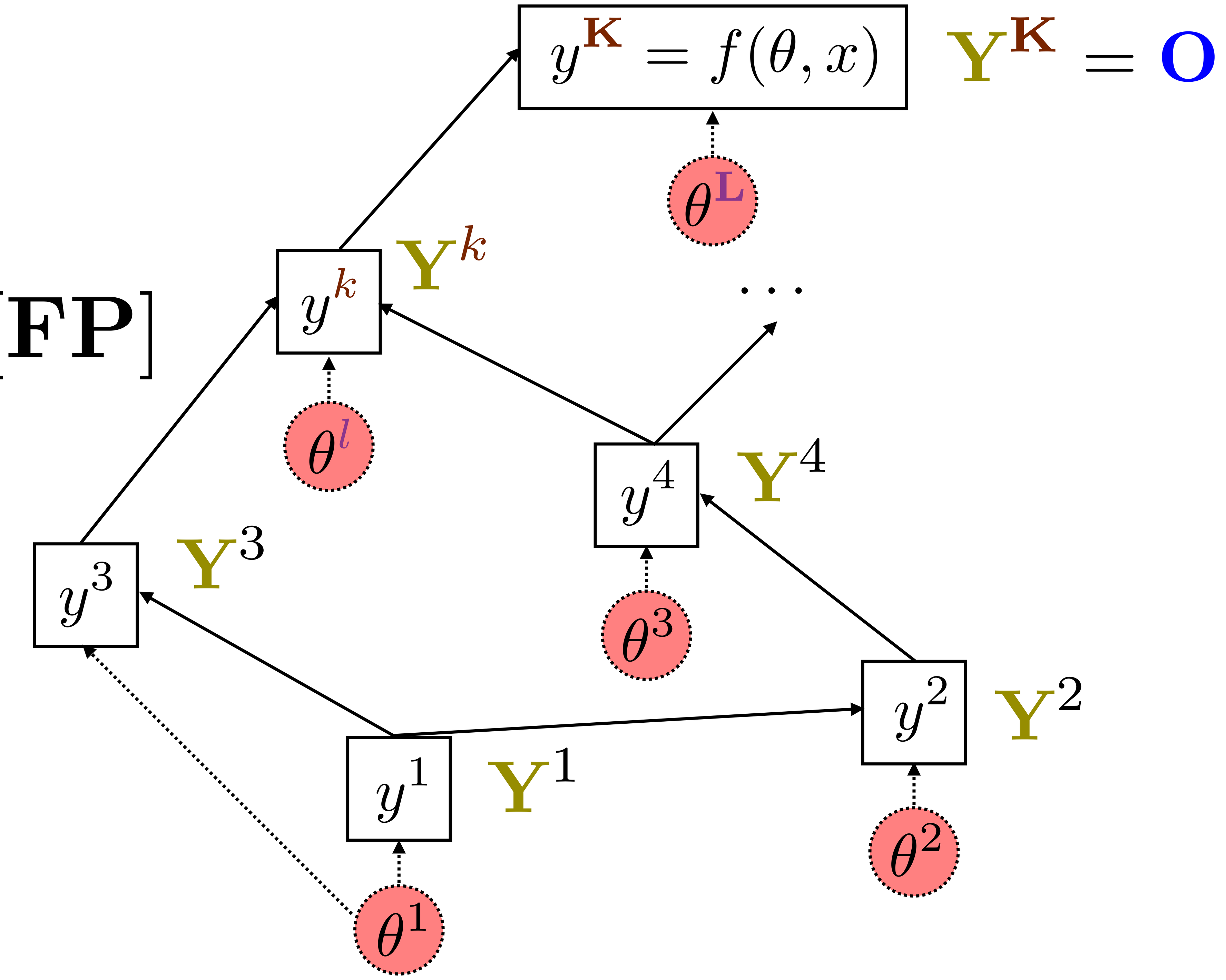
Idea 2: Structured derivatives

Consider the computation graph of the function f:

Forward Pass $[\mathbf{FP}]$

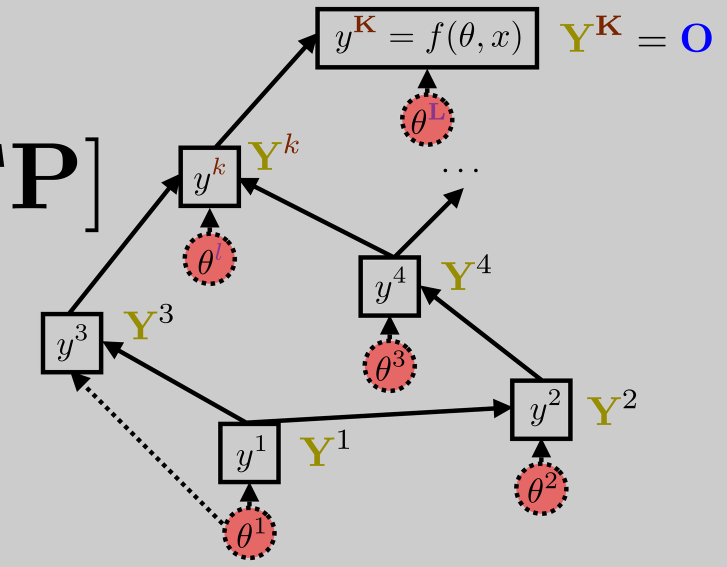


$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta} \frac{\partial f_2}{\partial \theta}^T$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \dots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \dots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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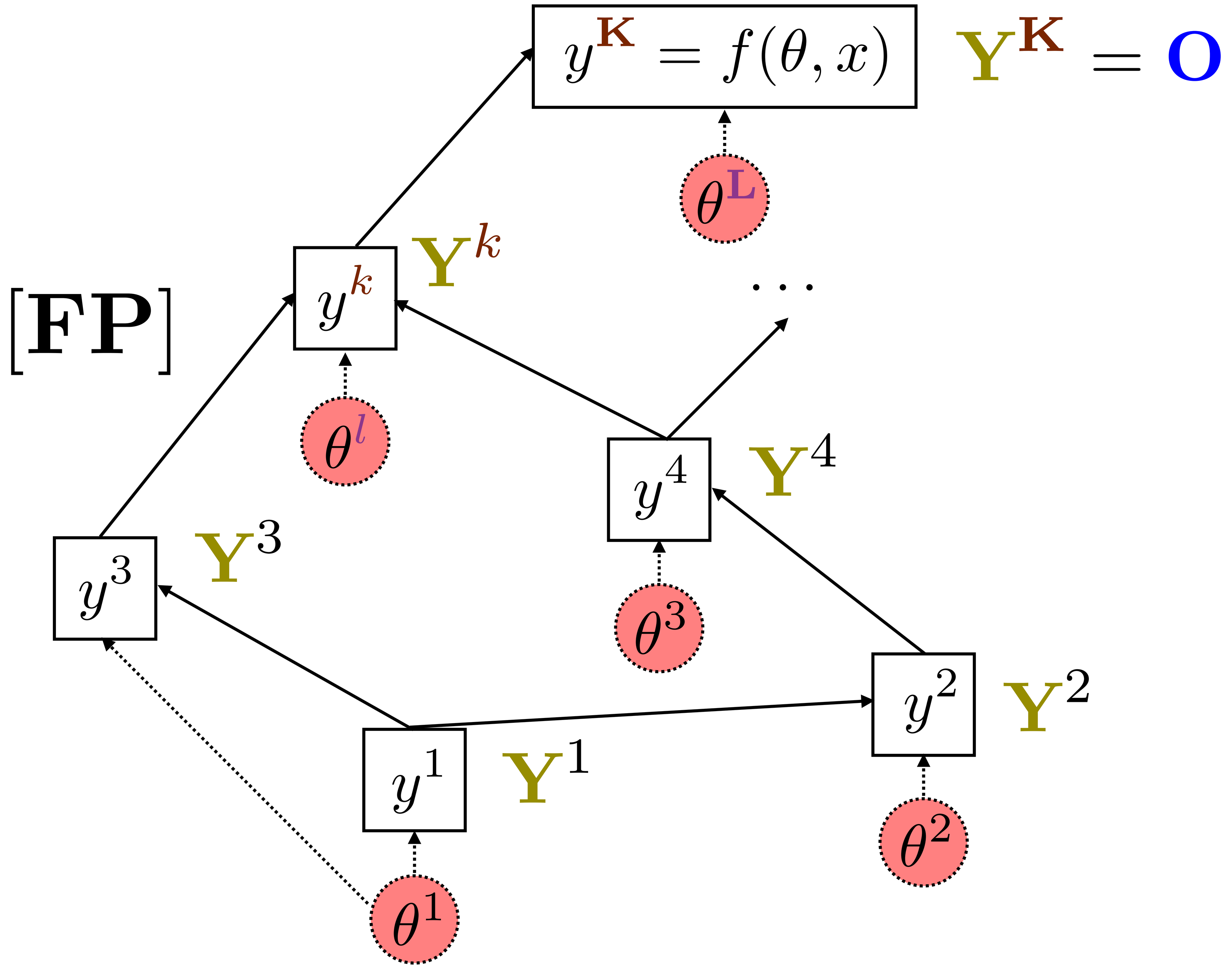
Idea 2: Structured derivatives

Apply the chain rule to the NTK expression:

Forward Pass $[\mathbf{FP}]$

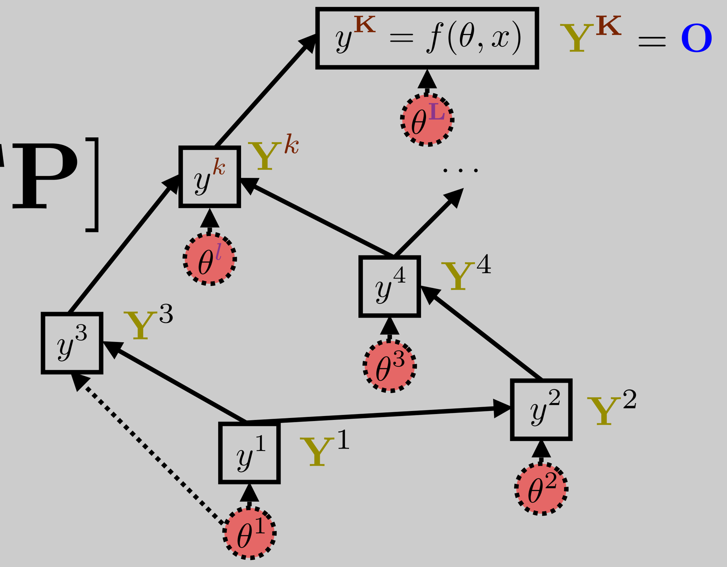


$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta} \frac{\partial f_2}{\partial \theta}^T = \sum_{l=0}^{\mathbf{L}} \frac{\partial f_1}{\partial \theta^l} \frac{\partial f_2}{\partial \theta^l}^T =$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



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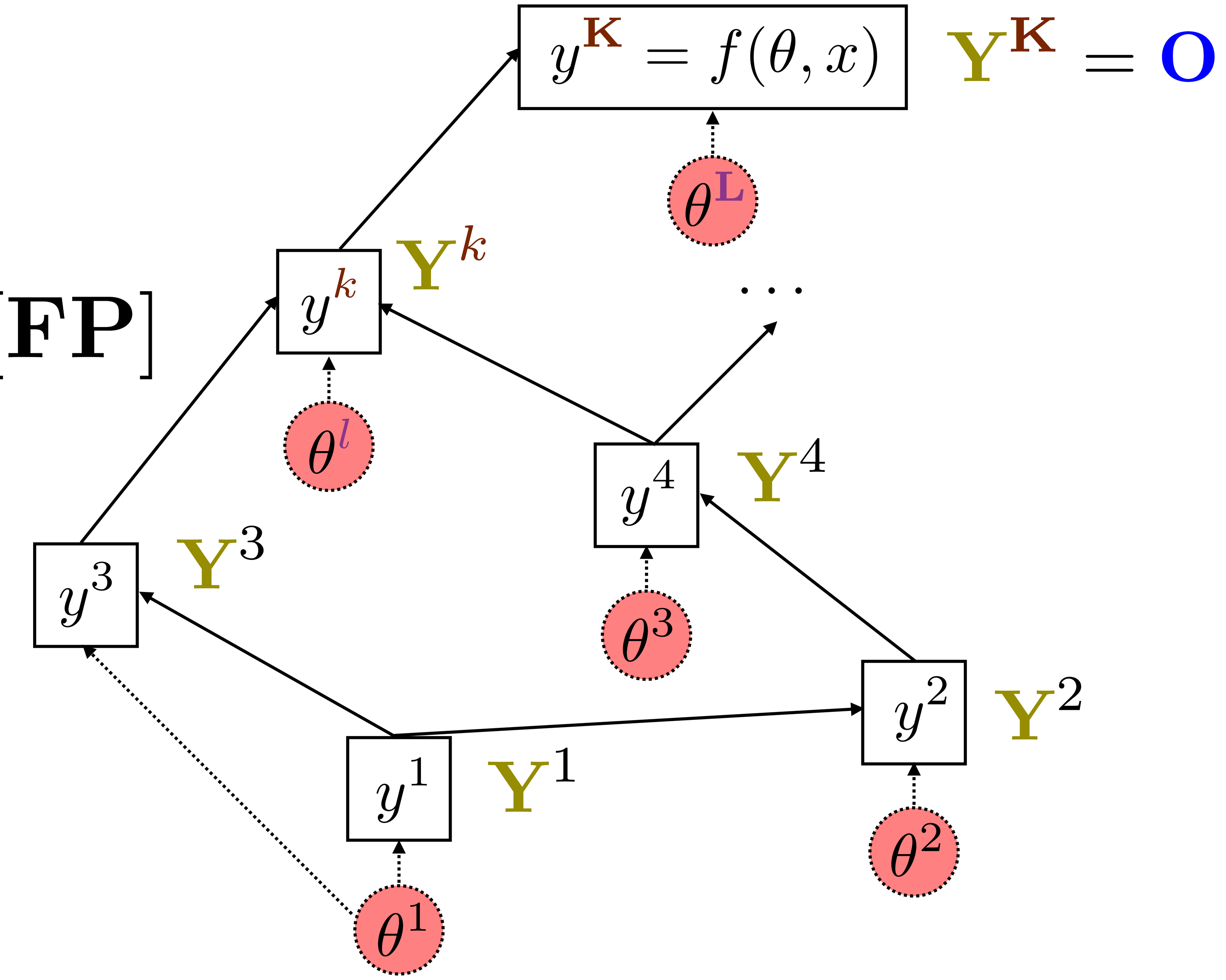
Forward Pass $[\mathbf{FP}]$



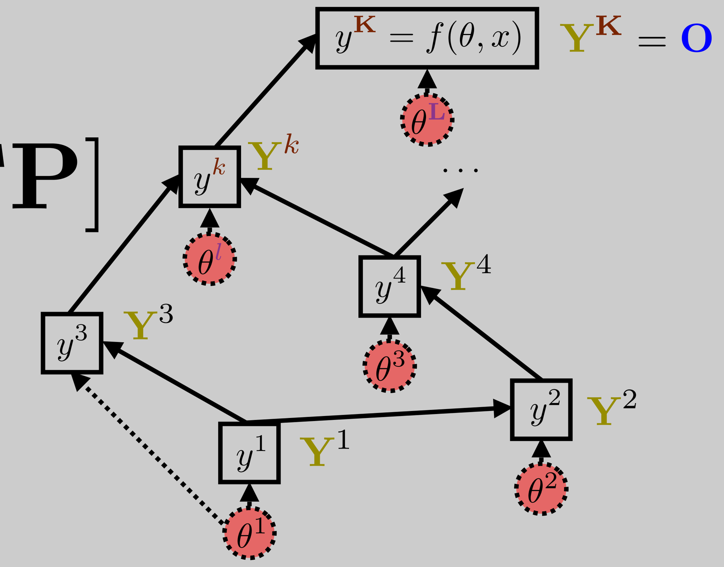
$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta} \frac{\partial f_2}{\partial \theta}^T = \sum_{l=0}^{\mathbf{L}} \frac{\partial f_1}{\partial \theta^l} \frac{\partial f_2}{\partial \theta^l}^T =$$

$$= \sum_{l, k_1, k_2} \left(\frac{\partial f_1}{\partial y_1^{k_1}} \frac{\partial y_1^{k_1}}{\partial \theta^l} \right) \left(\frac{\partial f_2}{\partial y_2^{k_2}} \frac{\partial y_2^{k_2}}{\partial \theta^l} \right)^T =$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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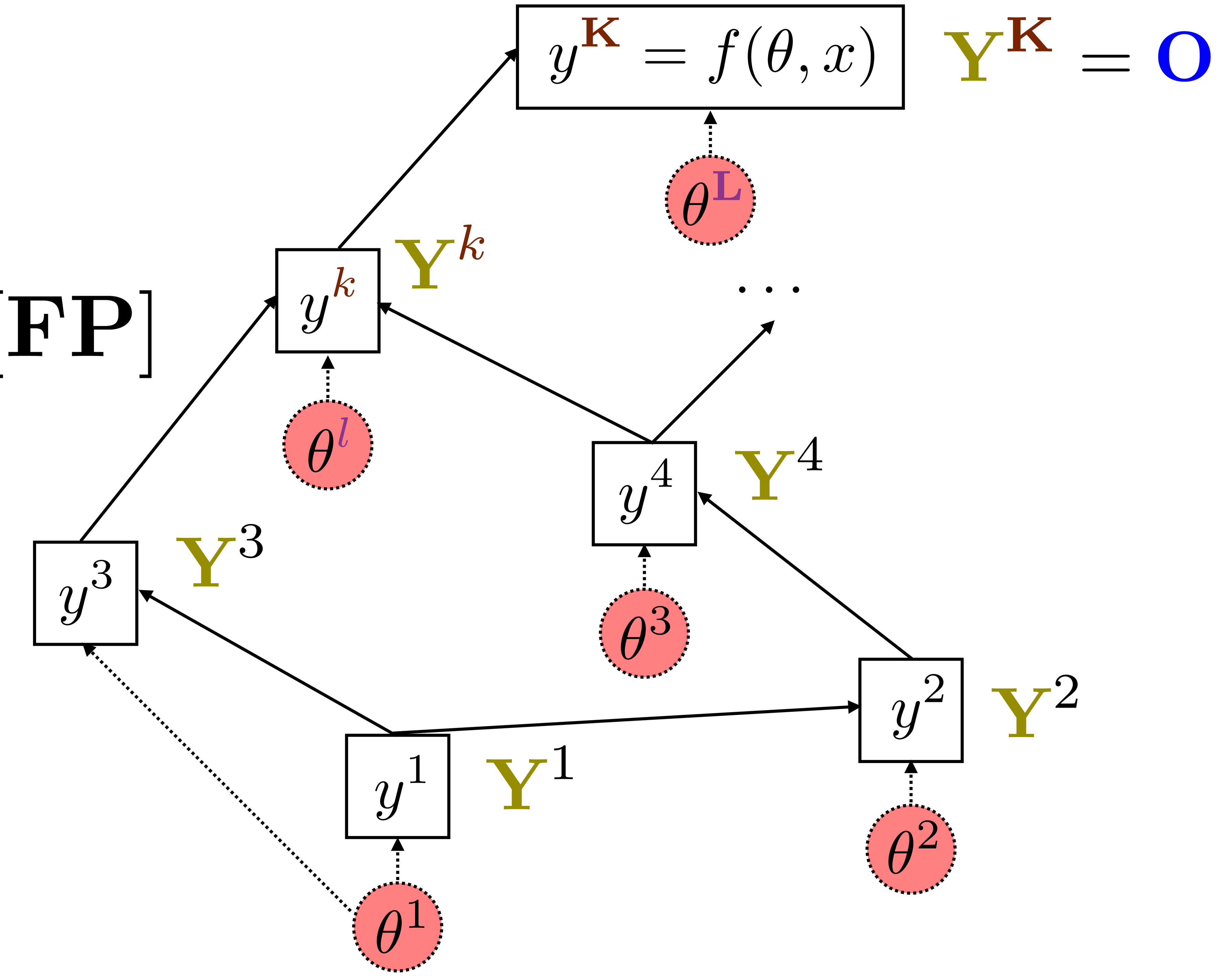
Apply the chain rule to the NTK expression:

Forward Pass $[\mathbf{FP}]$



$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta}\frac{\partial f_2}{\partial \theta}^T = \sum_{l=0}^{\mathbf{L}} \frac{\partial f_1}{\partial \theta^l}\frac{\partial f_2}{\partial \theta^l}^T =$$

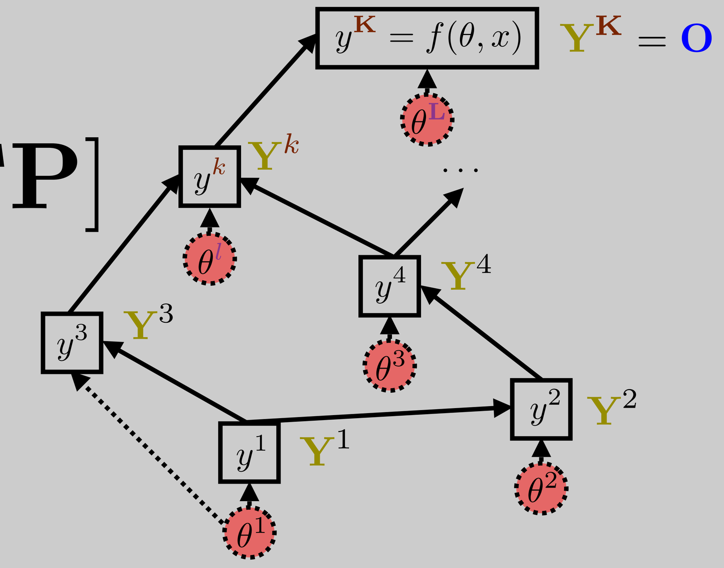
$$= \sum_{l, k_1, k_2} \left(\frac{\partial f_1}{\partial y_1^{k_1}}\frac{\partial y_1^{k_1}}{\partial \theta^l}\right)\left(\frac{\partial f_2}{\partial y_2^{k_2}}\frac{\partial y_2^{k_2}}{\partial \theta^l}\right)^T =$$

$$= \sum_{l, k_1, k_2} \frac{\partial f_1}{\partial y_1^{k_1}}\frac{\partial y_1^{k_1}}{\partial \theta^l}\frac{\partial y_2^{k_2}}{\partial \theta^l}^T \frac{\partial f_2}{\partial y_2^{k_2}}^T$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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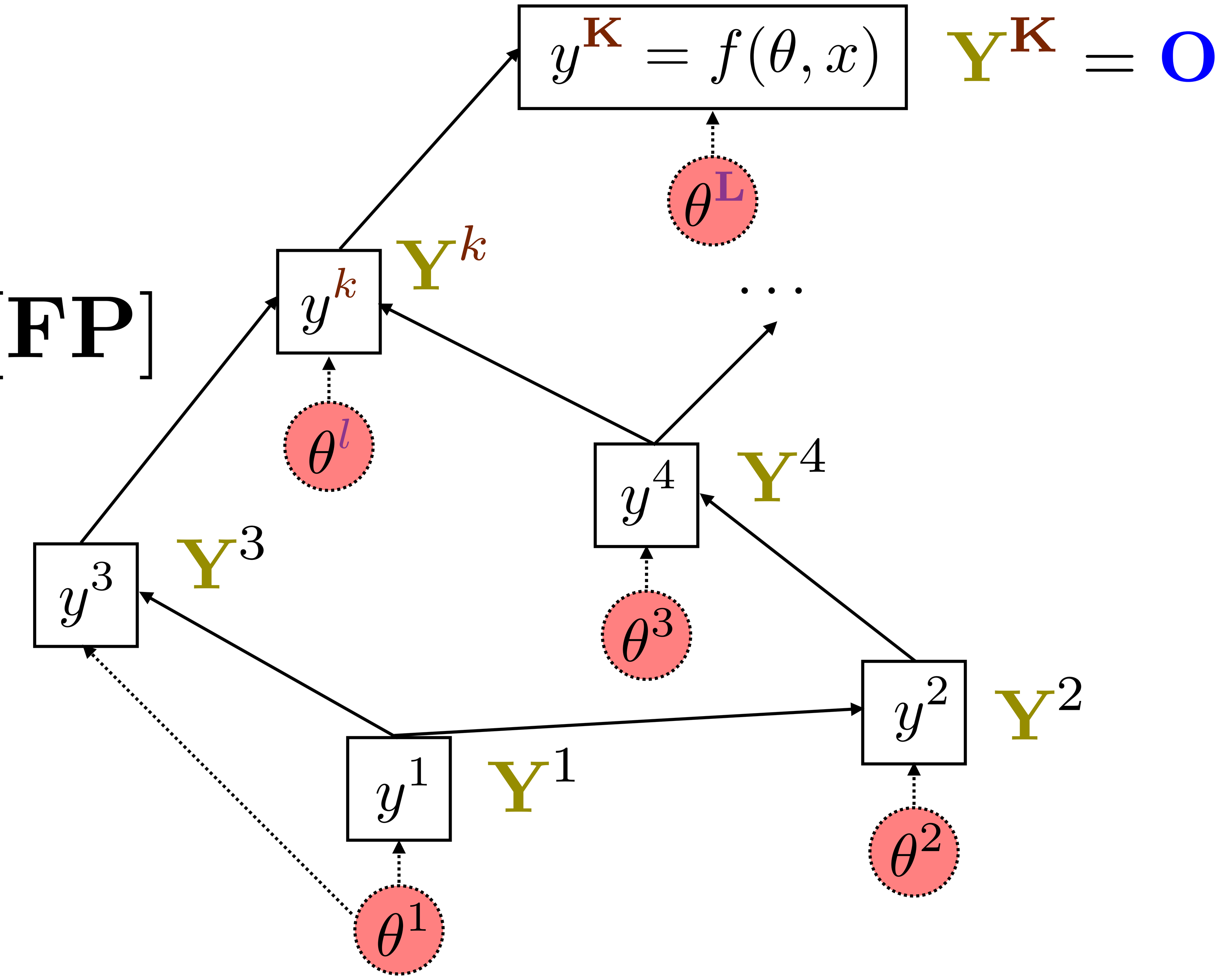
Idea 2: Structured derivatives

Apply the chain rule to the NTK expression:

Forward Pass $[\mathbf{FP}]$



$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta} \frac{\partial f_2}{\partial \theta}^T = \sum_{l=0}^{\mathbf{L}} \frac{\partial f_1}{\partial \theta^l} \frac{\partial f_2}{\partial \theta^l}^T =$$

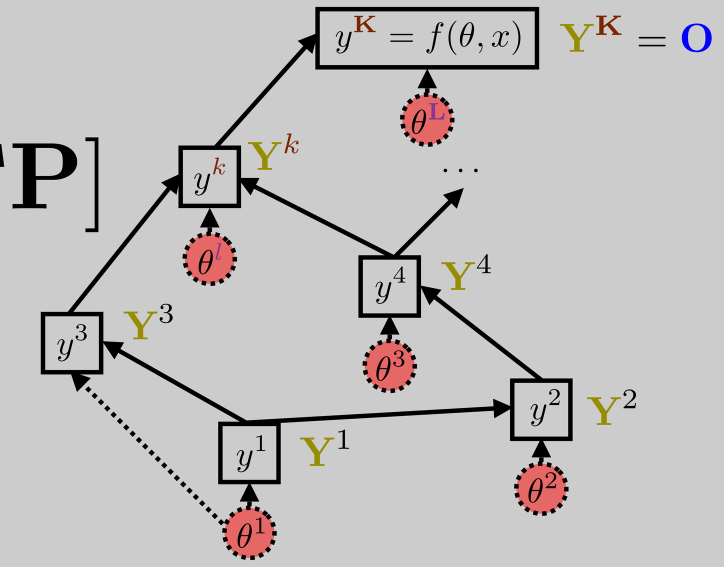
$$= \sum_{l,k_1,k_2} \left(\frac{\partial f_1}{\partial y_1^{k_1}} \frac{\partial y_1^{k_1}}{\partial \theta^l} \right) \left(\frac{\partial f_2}{\partial y_2^{k_2}} \frac{\partial y_2^{k_2}}{\partial \theta^l} \right)^T =$$

$$= \sum_{l,k_1,k_2} \frac{\partial f_1}{\partial y_1^{k_1}} \frac{\partial y_1^{k_1}}{\partial \theta^l} \frac{\partial y_2^{k_2}}{\partial \theta^l}^T \frac{\partial f_2}{\partial y_2^{k_2}}^T$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \dots, \theta^{\mathbf{L}}\right],$ $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \dots, y^{\mathbf{K}},$ $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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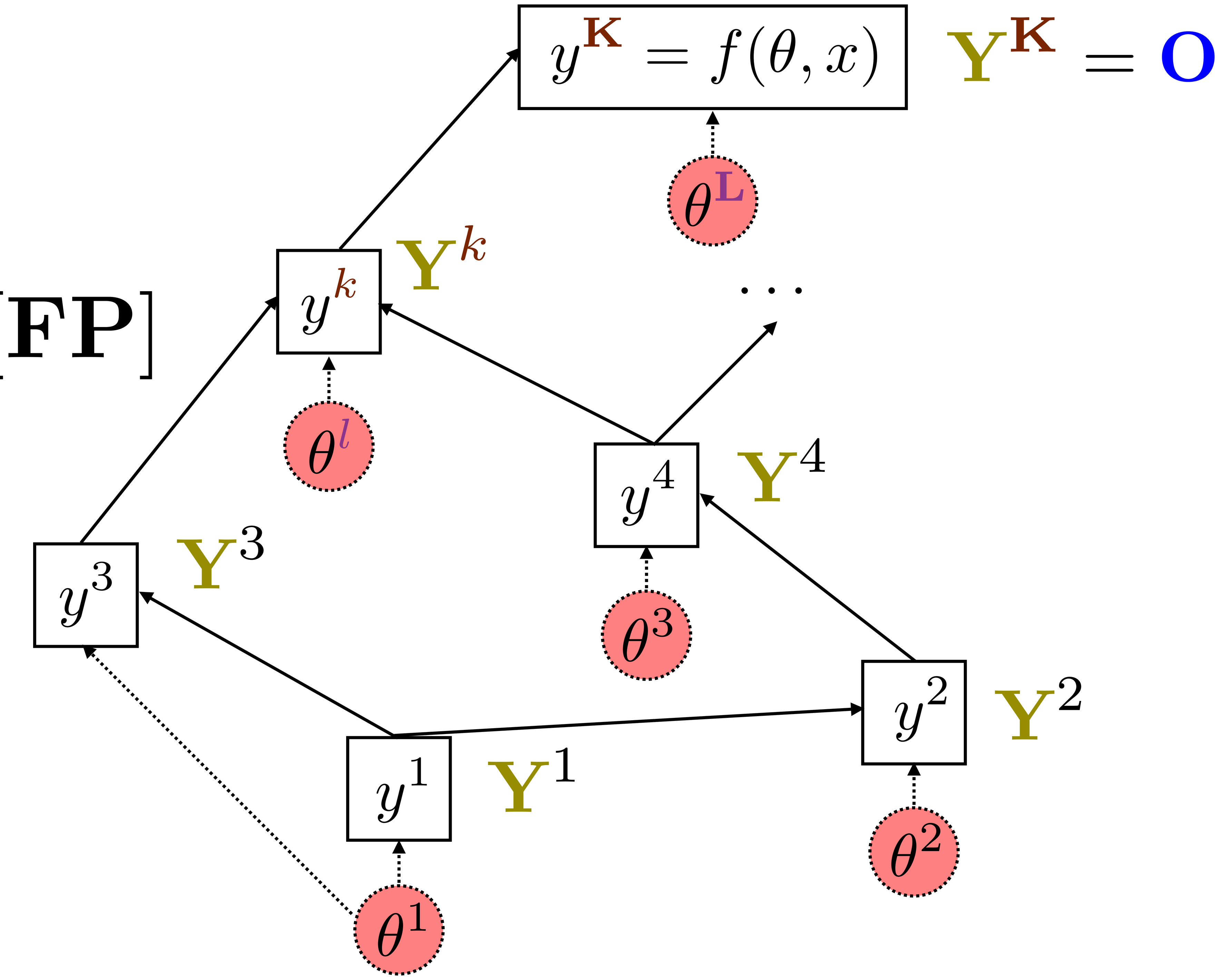
Idea 2: Structured derivatives

NTK is a sum of matrix-Jacobian-Jacobian-matrix products.

Forward Pass $[\mathbf{FP}]$



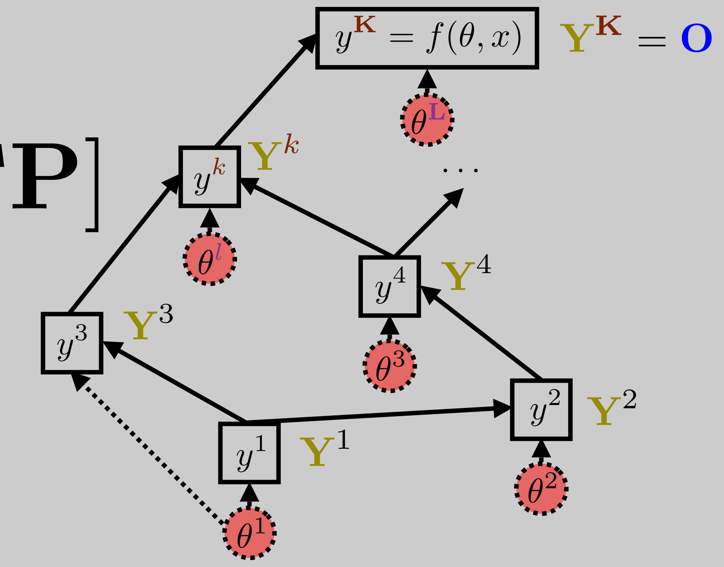
$$\Theta_\theta(x_1, x_2) = \frac{\partial f_1}{\partial \theta}\frac{\partial f_2}{\partial \theta}^T = \sum_{l=0}^{\mathbf{L}} \frac{\partial f_1}{\partial \theta^l}\frac{\partial f_2}{\partial \theta^l}^T = \sum_{l,k_1,k_2}\left(\frac{\partial f_1}{\partial y_1^{k_1}}\frac{\partial y_1^{k_1}}{\partial \theta^l}\right)\left(\frac{\partial f_2}{\partial y_2^{k_2}}\frac{\partial y_2^{k_2}}{\partial \theta^l}\right)^T$$

"matrix-Jacobian-Jacobian-matrix product" (MJJMP)

$$= \sum_{l,k_1,k_2} \frac{\partial f_1}{\partial y_1^{k_1}}\frac{\partial y_1^{k_1}}{\partial \theta^l}\frac{\partial y_2^{k_2}}{\partial \theta^l}^T\frac{\partial f_2}{\partial y_2^{k_2}}^T$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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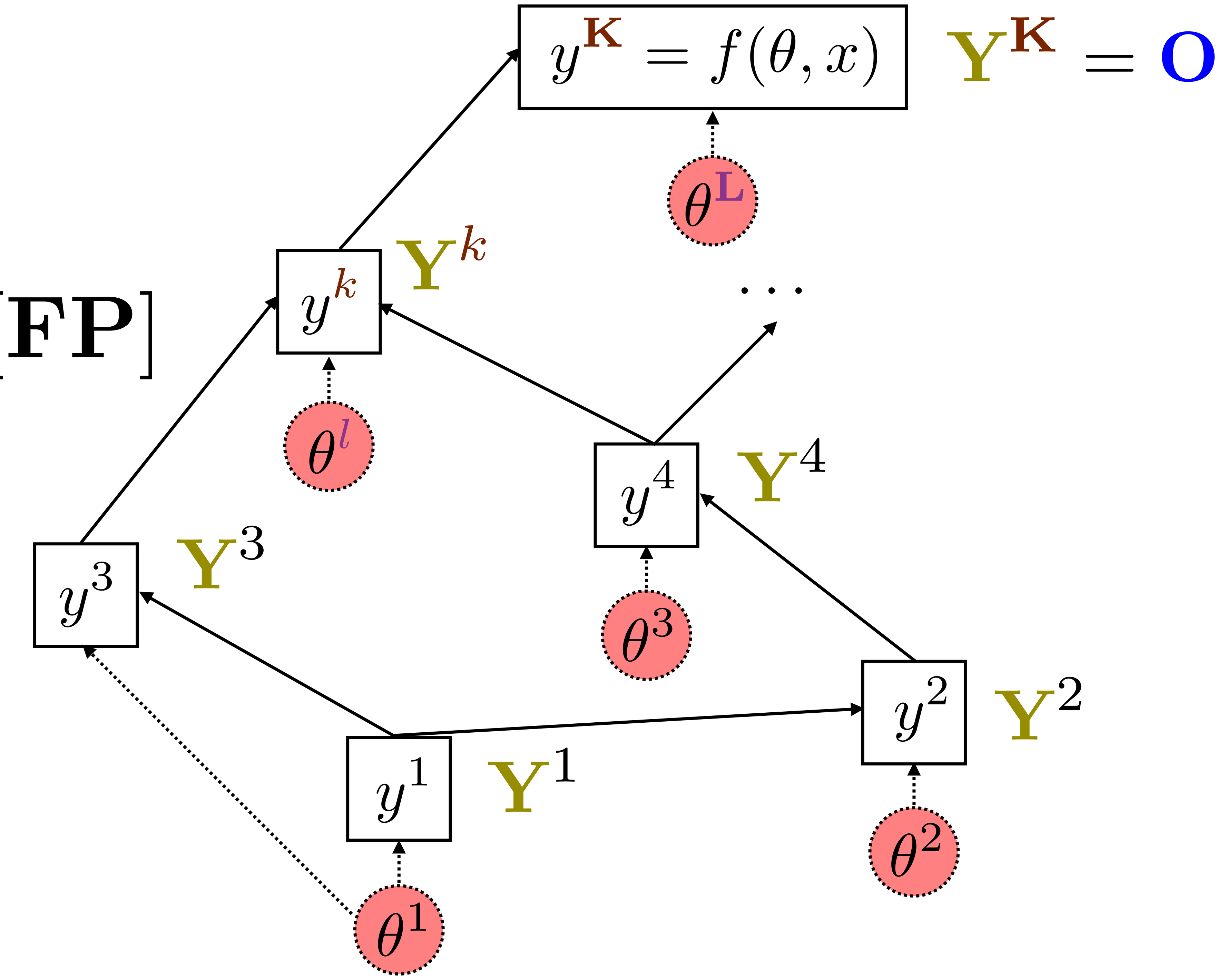
Idea 2: Structured derivatives

Idea: for every pair of primitives y_1, y_2, implement efficient MJJMPs:

Forward Pass $[\mathbf{FP}]$



$$\Big(\underbrace{c_1}_{\mathbf{O}\times\mathbf{Y}_1}, \underbrace{c_2}_{\mathbf{O}\times\mathbf{Y}_2}\Big) \mapsto \underbrace{c_1 \frac{\partial y_1}{\partial \theta} \frac{\partial y_2}{\partial \theta}^T c_2^T}_{\mathbf{O}\times\mathbf{O}}$$

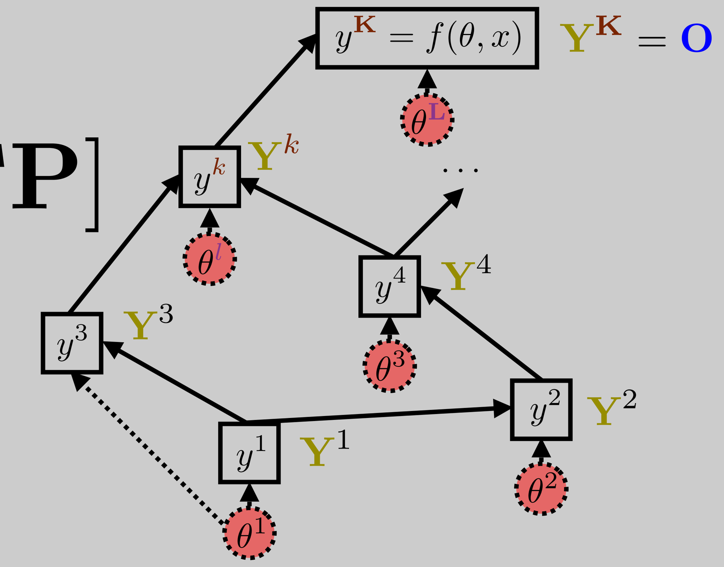
"matrix-Jacobian-Jacobian-matrix product" (MJJMP)

$$= \sum_{l,k_1,k_2} \frac{\partial f_1}{\partial y_1^{k_1}} \frac{\partial y_1^{k_1}}{\partial \theta^l} \frac{\partial y_2^{k_2}}{\partial \theta^l}^T \frac{\partial f_2}{\partial y_2^{k_2}}^T$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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Idea 2: Structured derivatives

Idea: for every pair of primitives y_1, y_2, implement efficient **MJJMPs**:

$$\Big(\underbrace{c_1}_{\mathbf{O}\times\mathbf{Y}_1}, \underbrace{c_2}_{\mathbf{O}\times\mathbf{Y}_2}\Big) \mapsto \underbrace{c_1 \frac{\partial y_1}{\partial \theta} \frac{\partial y_2}{\partial \theta}^T c_2^{\,T}}_{\mathbf{O}\times\mathbf{O}}$$

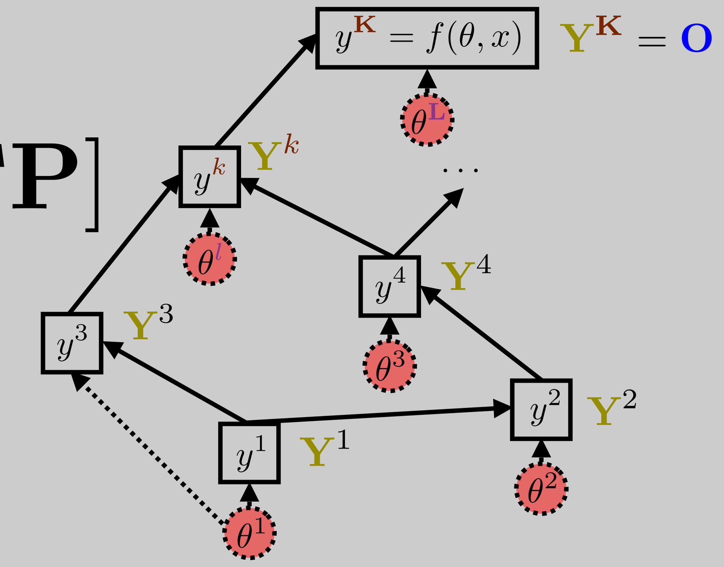
Similar to existing AD tools: for every primitive y, implement efficient

$$\mathrm{JVP}_{(y,\theta)} : \theta_t \in \mathbb{R}^{\mathbf{P}} \mapsto \frac{\partial y}{\partial \theta}\theta_t \in \mathbb{R}^{\mathbf{Y}} \qquad \mathrm{VJP}_{(y,\theta)} : y_c \in \mathbb{R}^{\mathbf{Y}} \mapsto \frac{\partial y}{\partial \theta}^T y_c \in \mathbb{R}^{\mathbf{P}}$$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

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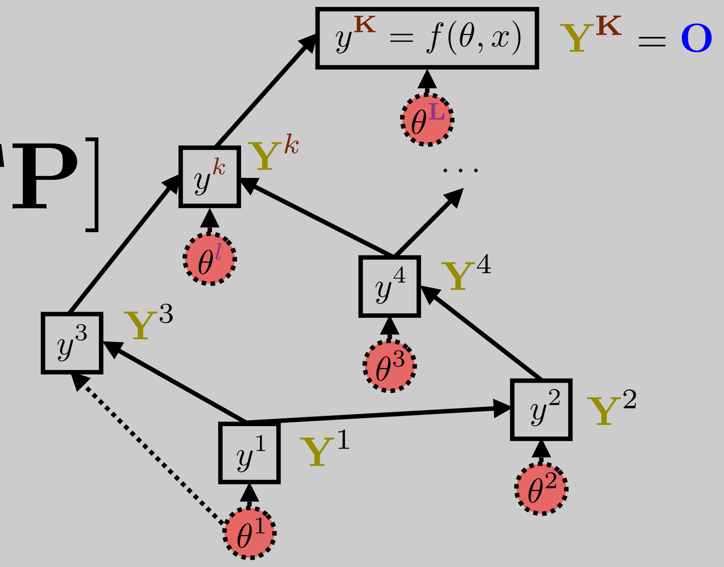
Methods summary

Method	Jacobian Contraction	NTK-vector products	Structured derivatives
Time	$\mathbf{N}\mathbf{O}\,[\mathbf{FP}] + \mathbf{N}^2\mathbf{O}^2\mathbf{P}$	$\mathbf{N}^2\mathbf{O}\,[\mathbf{FP}]$	$\mathbf{N}\mathbf{O}\,[\mathbf{FP}] + \mathbf{MJJMP}$

Neural Network $f(\theta, x) \in \mathbb{R}^{\mathbf{O}}$

Forward Pass $[\mathbf{FP}]$



Parameters $\theta = \mathrm{vec}\left[\theta^0, \ldots, \theta^{\mathbf{L}}\right]$, $\mathbf{P} = \sum_{l=0}^{\mathbf{L}} \mathbf{P}^l$

Batch size $\mathbf{N}$ Output size $\mathbf{O}$

Intermediate primitive outputs $y^1, \ldots, y^{\mathbf{K}}$, $\mathbf{Y} = \sum_{k=1}^{\mathbf{K}} \mathbf{Y}^k$

Plan

1. NTK definition and notation
2. Recap of Automatic Differentiation (AD)
3. Baseline NTK computation complexity
4. Two new algorithms for computing the NTK
5. **Benchmarks**

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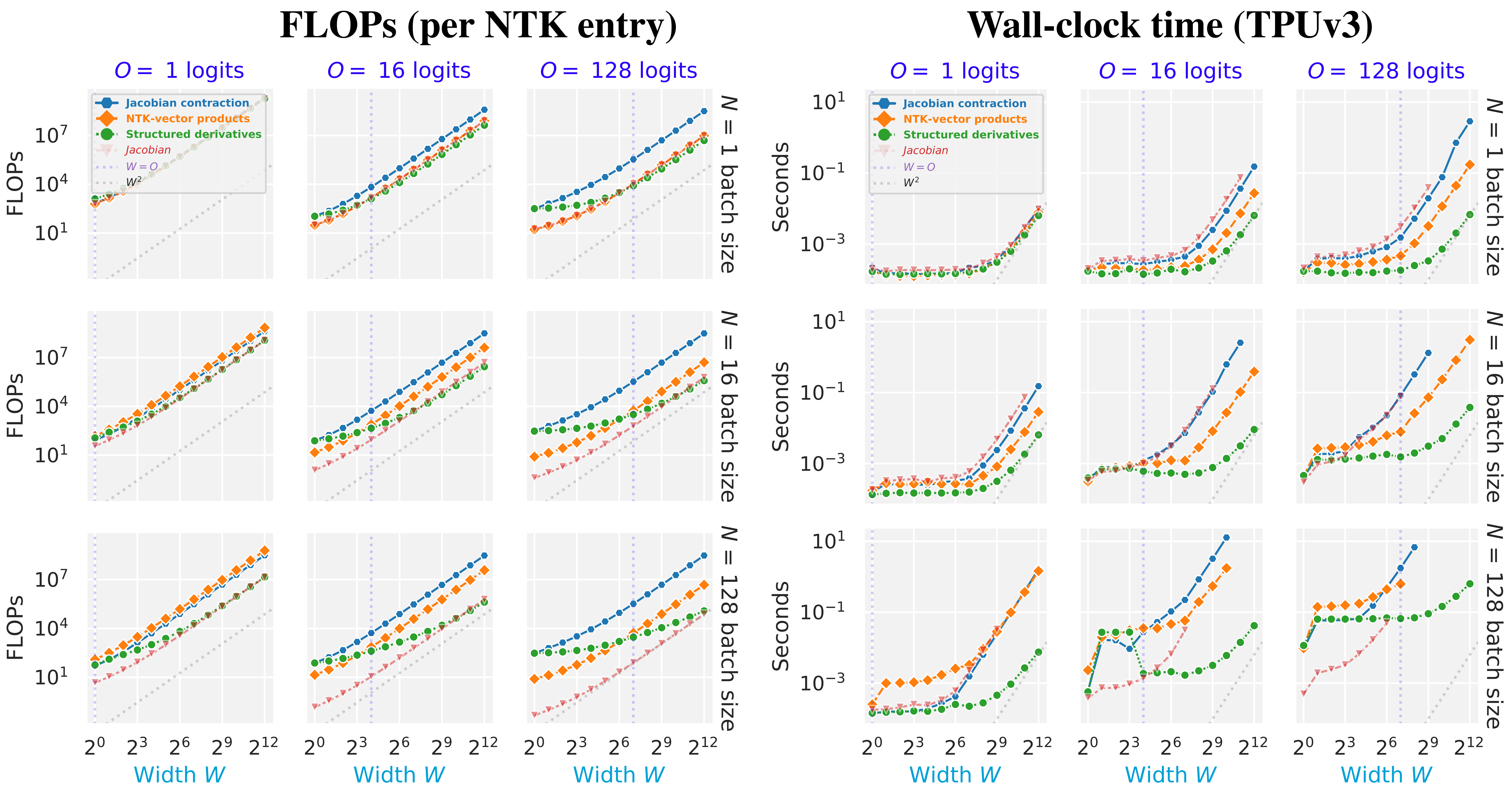
Benchmarks on FCNs



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Benchmarks on ImageNet ResNets

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ImageNet Transformers/Mixers/Hybrids

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2-line code sample

```
pip install neural_tangents
```

```
import neural_tangents as nt


# Given any f: params, x -> f(params, x)
ntk_fn = nt.empirical_ntk_fn(f, implementation=1)  # 1, 2, or 3
ntk = ntk_fn(x1, x2, params)
```

github.com/google/neural-tangents


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