Cross-Validation

A Fast Algorithm by

Ole-Christian Galbo Engstrøm and Martin Holm Jensen

K

M

N

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

N

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

K

N

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

M

N

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

K

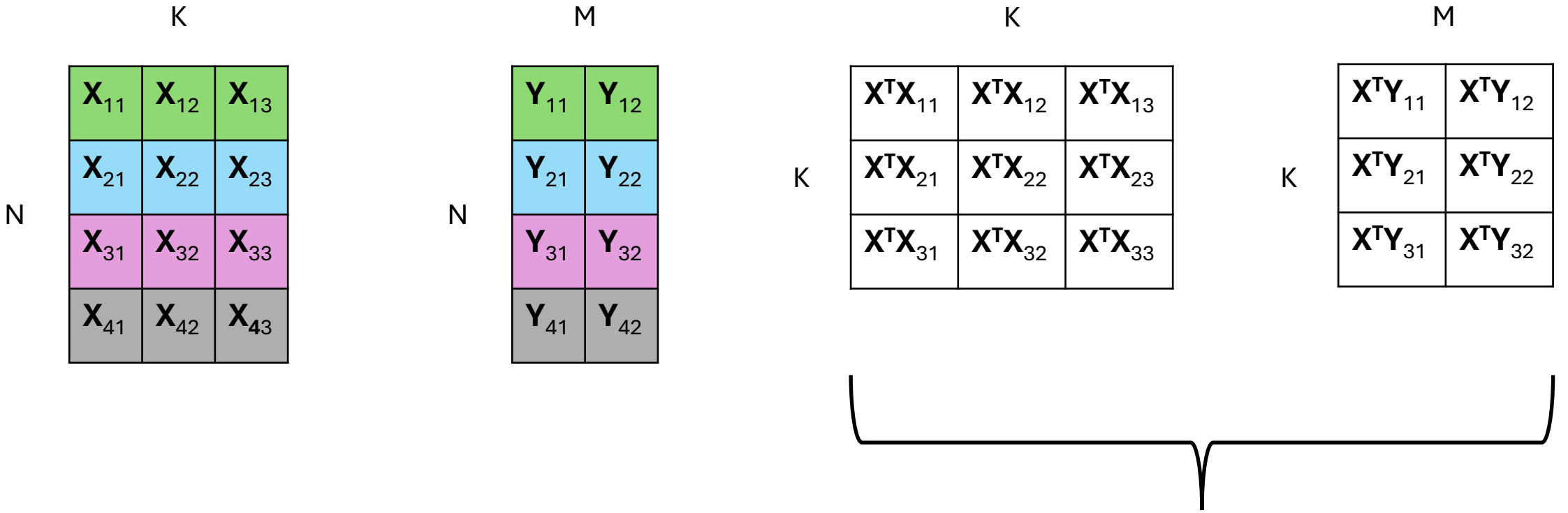
K

X^TX_{11}	X^TX_{12}	X^TX_{13}
X^TX_{21}	X^TX_{22}	X^TX_{23}
X^TX_{31}	X^TX_{32}	X^TX_{33}

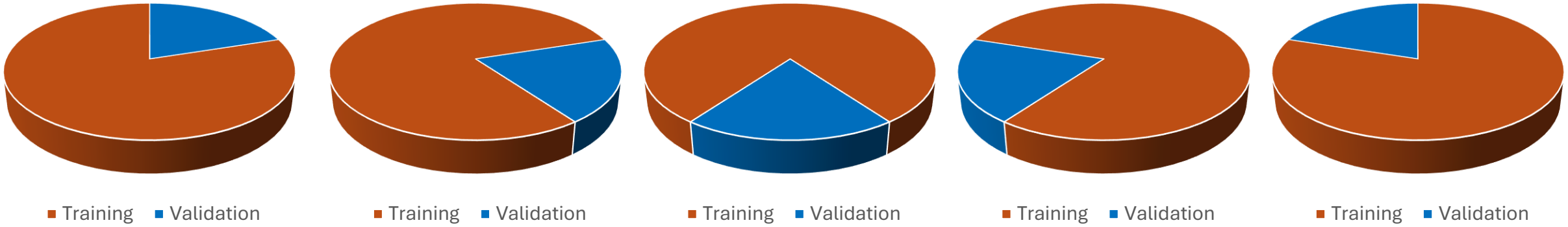
M

K

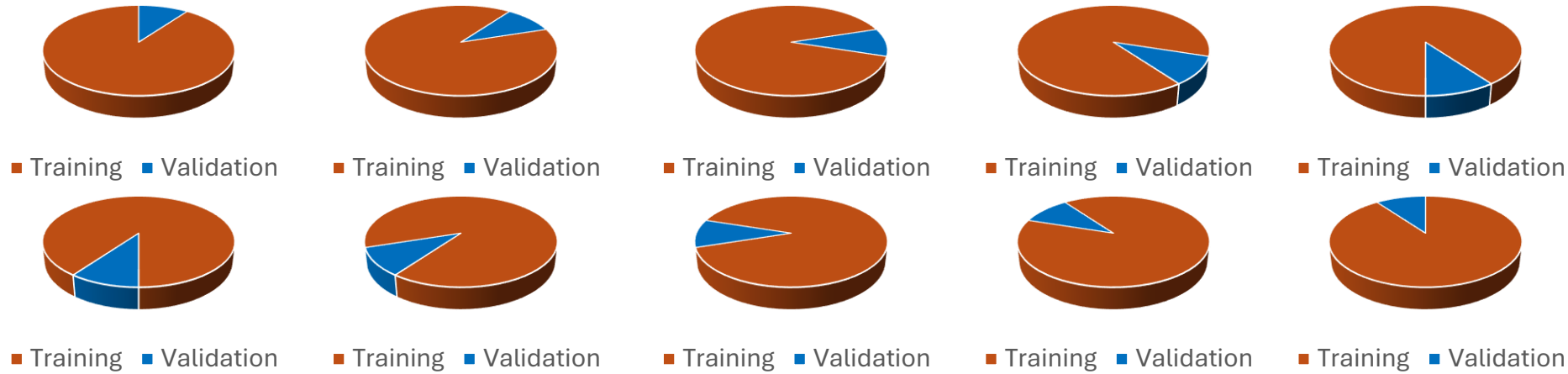
X^TY_{11}	X^TY_{12}
X^TY_{21}	X^TY_{22}
X^TY_{31}	X^TY_{32}


K
M
K
M
N
N
K
K
X_{11} X_{12} X_{13}
X_{21} X_{22} X_{23}
X_{31} X_{32} X_{33}
X_{41} X_{42} X_{43}
Y_{11} Y_{12}
Y_{21} Y_{22}
Y_{31} Y_{32}
Y_{41} Y_{42}
X^TX_{11} X^TX_{12} X^TX_{13}
X^TX_{21} X^TX_{22} X^TX_{23}
X^TX_{31} X^TX_{32} X^TX_{33}
X^TY_{11} X^TY_{12}
X^TY_{21} X^TY_{22}
X^TY_{31} X^TY_{32}
Ordinary/Partial Least Squares
Ridge Regression
Principal Component Analysis/Regression
Etc.

5-fold cross-validation



10-fold cross-validation



Total number of samples: NP

Total number of validation samples: N

Total number of training samples: $NP - N = N(P-1) = \Theta(NP)$

X

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

Y

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

X^T

X_{11}	X_{21}	X_{31}	X_{41}
X_{12}	X_{22}	X_{32}	X_{42}
X_{13}	X_{23}	X_{33}	X_{43}

X^TY

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

X

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

Y

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

Fold 1

X^T

X_{11}	X_{21}	X_{31}	X_{41}
X_{12}	X_{22}	X_{32}	X_{42}
X_{13}	X_{23}	X_{33}	X_{43}

X^TY_{Train}

$X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

Fold 2

X

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

Y

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

Training

Validation

X^T

X_{11}	X_{21}	X_{31}	X_{41}
X_{12}	X_{22}	X_{32}	X_{42}
X_{13}	X_{23}	X_{33}	X_{43}

X^TY_{Train}

$X_{11}Y_{11}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{33}Y_{32}+X_{43}Y_{42}$

Fold 3

X

X_{11}	X_{12}	X_{13}
X_{21}	X_{22}	X_{23}
X_{31}	X_{32}	X_{33}
X_{41}	X_{42}	X_{43}

Y

Y_{11}	Y_{12}
Y_{21}	Y_{22}
Y_{31}	Y_{32}
Y_{41}	Y_{42}

Training

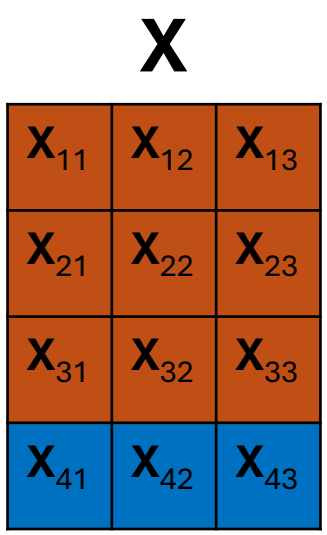
Validation

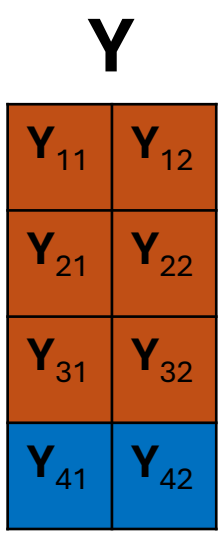
X^T

X_{11}	X_{21}	X_{31}	X_{41}
X_{12}	X_{22}	X_{32}	X_{42}
X_{13}	X_{23}	X_{33}	X_{43}

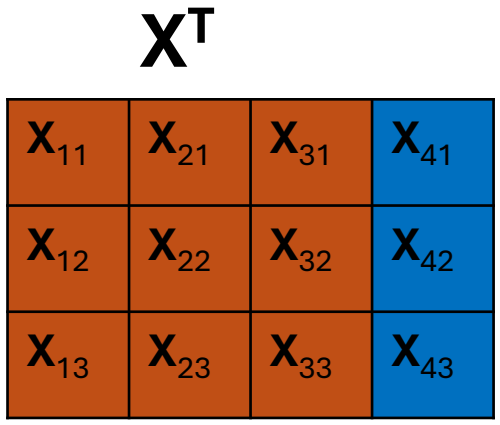
X^TY_{Train}

$X_{11}Y_{11}+X_{21}Y_{21}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{43}Y_{42}$





Fold 4



$X^T Y_{Train}$

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}$

N rows in **X** and **Y**

K columns in **X**

M columns in **Y**

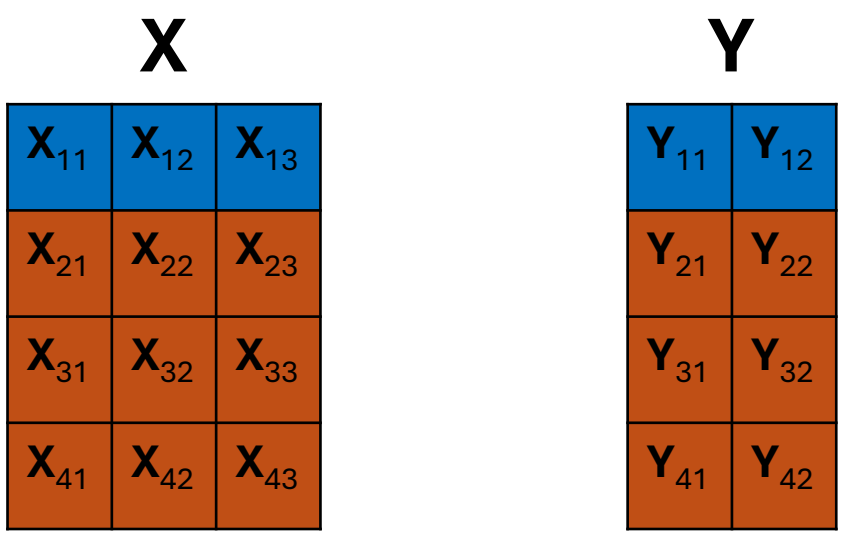
N rows in **X** and **Y**
K columns in **X**
M columns in **Y**

Each $\mathbf{X}^T\mathbf{Y}_{\text{Train}}$
Time: Θ(NKM)

P folds:
Time: Θ(PNKM)

... Can we do better?

$$X^T Y_{Train} = X^T Y - X^T Y_{Val}$$



Fold 1

$X^T Y_{Train}$

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}$

=

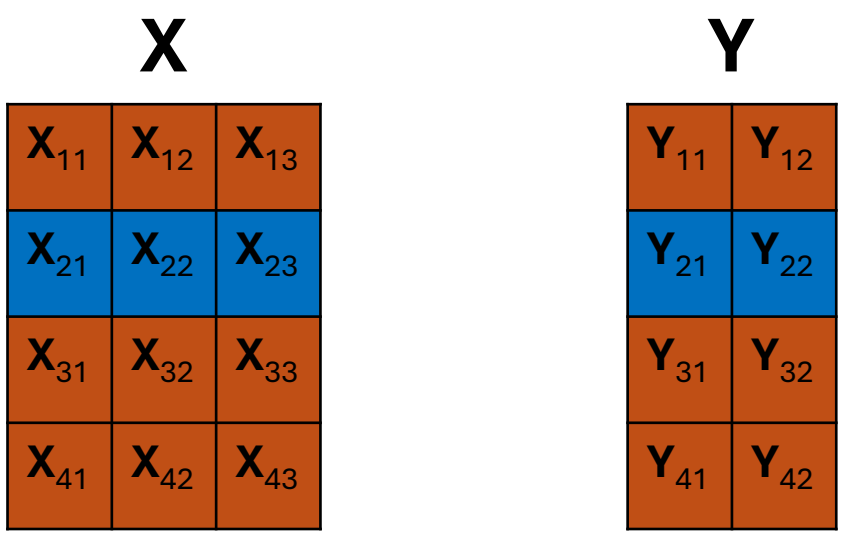
$X^T Y$

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

-

$X^T Y_{Val}$

$X_{11}Y_{11}$	$X_{11}Y_{12}$
$X_{12}Y_{11}$	$X_{12}Y_{12}$
$X_{13}Y_{11}$	$X_{13}Y_{12}$



Fold 2

Training

Validation

X^TY_{Train}

$X_{11}Y_{11}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}$

=

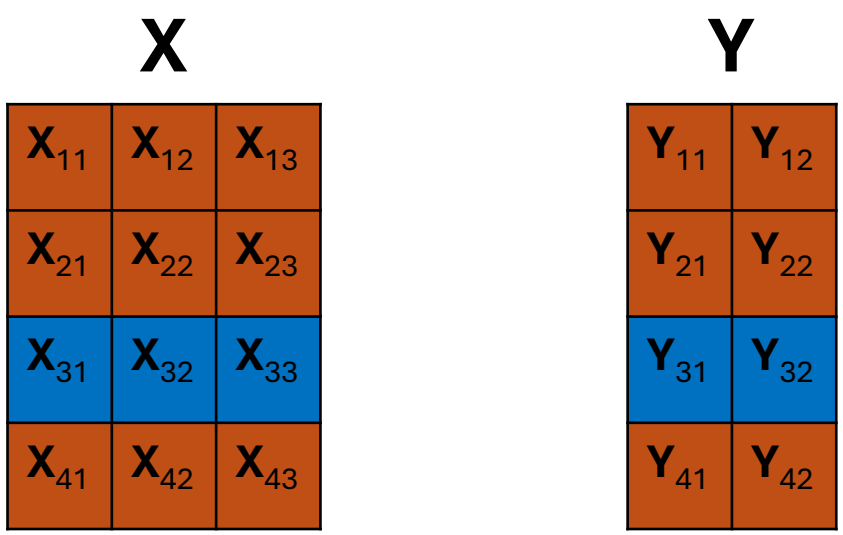
X^TY

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

-

X^TY_{Val}

$X_{21}Y_{21}$	$X_{21}Y_{22}$
$X_{22}Y_{21}$	$X_{22}Y_{22}$
$X_{23}Y_{21}$	$X_{23}Y_{22}$



Fold 3

Training

Validation

X^TY_{Train}

$X_{11}Y_{11}+X_{21}Y_{21}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{43}Y_{42}$

=

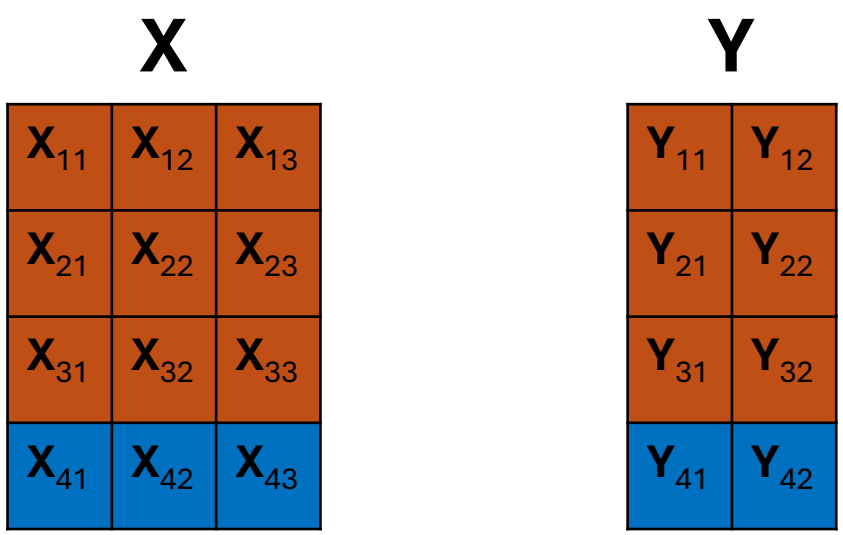
X^TY

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

-

X^TY_{Val}

$X_{31}Y_{31}$	$X_{31}Y_{32}$
$X_{32}Y_{31}$	$X_{32}Y_{32}$
$X_{33}Y_{31}$	$X_{33}Y_{32}$



Fold 4

Training

Validation

X^TY_{Train} = X^TY - X^TY_{Val}

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}$	$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$	$X_{41}Y_{41}$	$X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}$	$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$	$X_{42}Y_{41}$	$X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}$	$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$	$X_{43}Y_{41}$	$X_{43}Y_{42}$

$$X^TY_{Train} = X^TY - X^TY_{Val}$$

Once:

X^TY

P times:

X^TY_{Val}

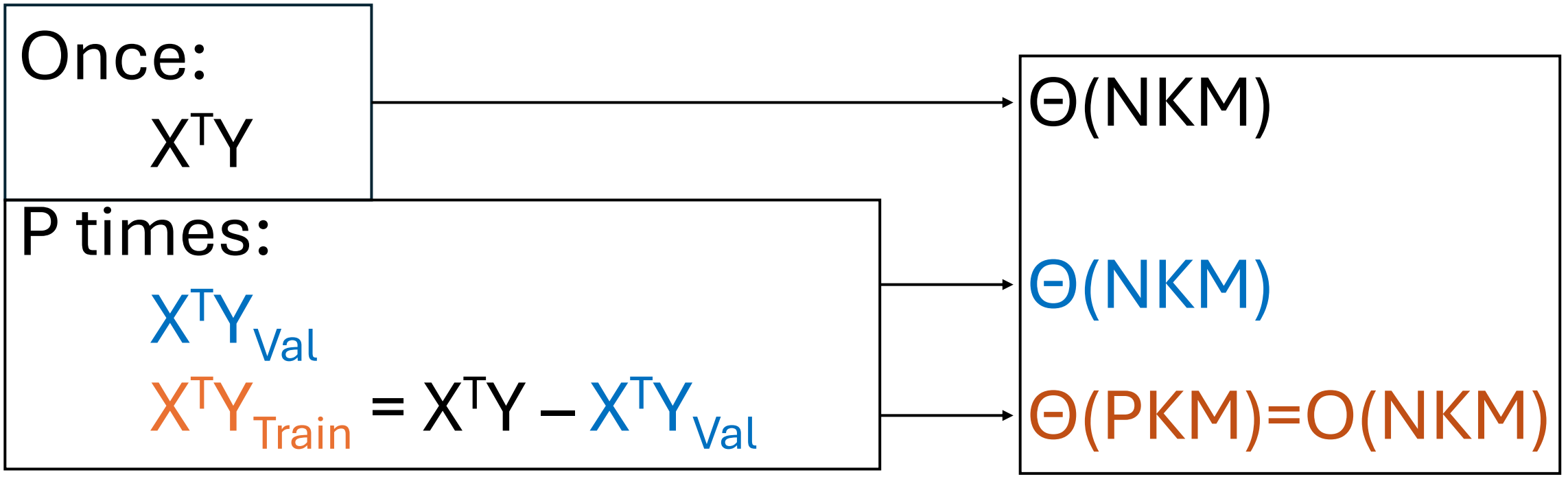
$X^TY_{Train} = X^TY - X^TY_{Val}$

$X^TY_{Train} = X^TY - X^TY_{Val}$

N rows in **X** and **Y**

K columns in **X**

M columns in **Y**

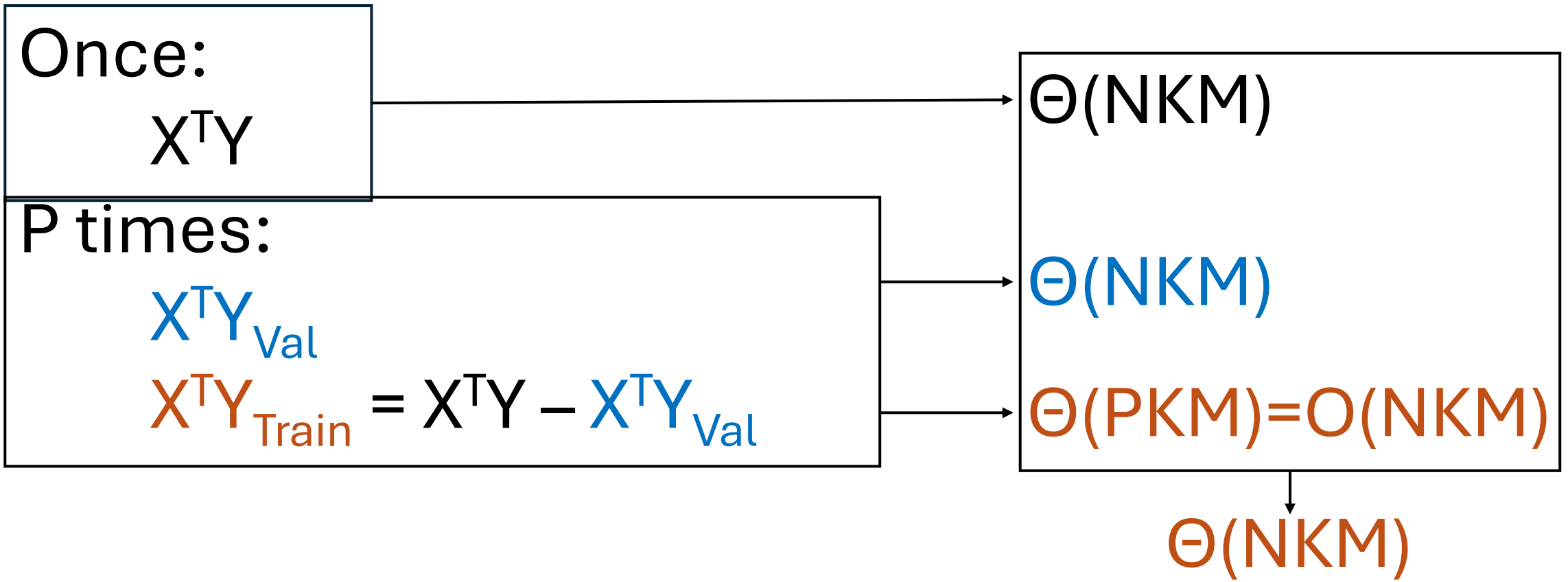


$X^TY_{Train} = X^TY - X^TY_{Val}$

N rows in **X** and **Y**

K columns in **X**

M columns in **Y**



$X^TY_{Train} = X^TY - X^TY_{Val}$

N rows in **X** and **Y**

K columns in **X**

M columns in **Y**

Asymptotically independent on P!

Once:

X^TY

$\Theta(NKM)$

P times:

X^TY_{Val}

$\Theta(NKM)$

$X^TY_{Train} = X^TY - X^TY_{Val}$

$\Theta(PKM)=O(NKM)$

$\Theta(NKM)$

Cost of computing all P $X^T Y_{Train}$

Improved from Θ(PNKM) to Θ(NKM)

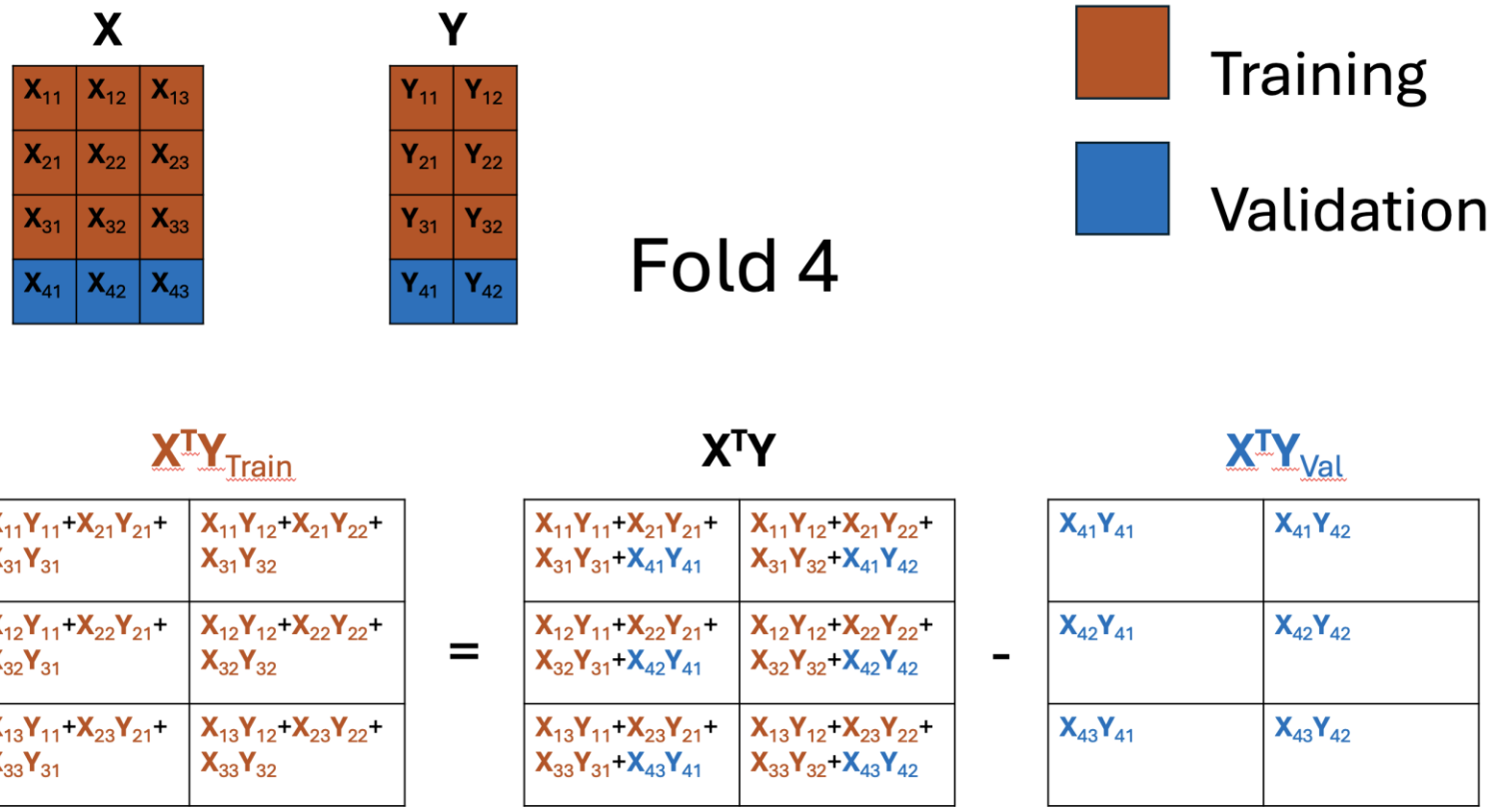
Cost of computing all P X^TY_{Train}
Improved from Θ(PNKM) to Θ(NKM)

Cost of computing all P X^TX_{Train}
Improved from Θ(PNKK) to Θ(NKK)

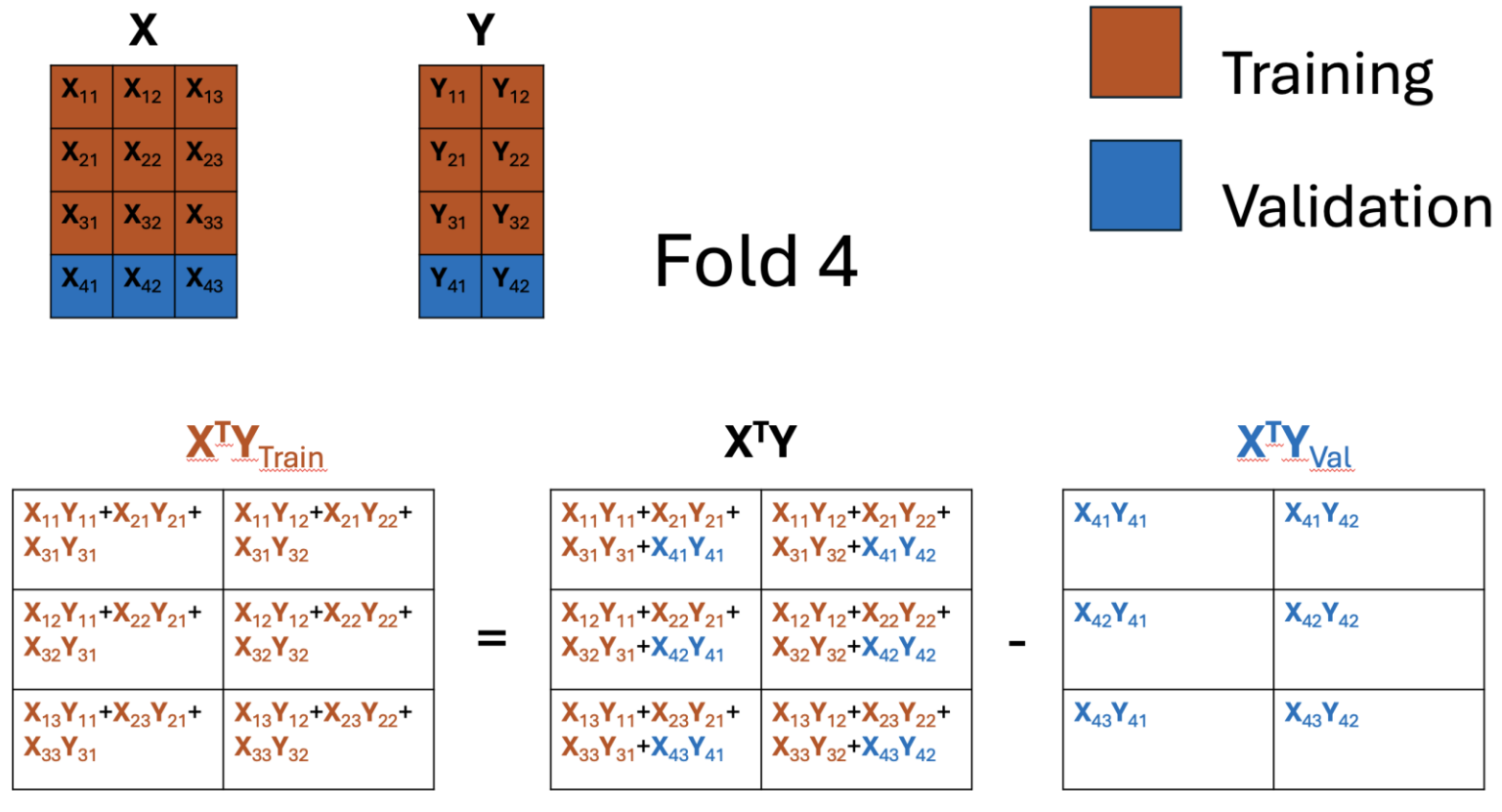
Cost of computing all P X^TY_{Train} and X^TX_{Train}
Improved from Θ(PNK(K+M)) to Θ(NK(K+M))

… Any row-wise preprocessing works out of the box

SNV, i.e., (row-wise) centering and scaling
Convolution (e.g. with Savitzky-Golay filters)



… What about (column-wise) centering and scaling (autoscaling)?



$$X^T Y_{Train} = X^T Y - X^T Y_{Val}$$

$X^T Y_{Train}$

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}$

=

$X^T Y$

$X_{11}Y_{11}+X_{21}Y_{21}+X_{31}Y_{31}+X_{41}Y_{41}$	$X_{11}Y_{12}+X_{21}Y_{22}+X_{31}Y_{32}+X_{41}Y_{42}$
$X_{12}Y_{11}+X_{22}Y_{21}+X_{32}Y_{31}+X_{42}Y_{41}$	$X_{12}Y_{12}+X_{22}Y_{22}+X_{32}Y_{32}+X_{42}Y_{42}$
$X_{13}Y_{11}+X_{23}Y_{21}+X_{33}Y_{31}+X_{43}Y_{41}$	$X_{13}Y_{12}+X_{23}Y_{22}+X_{33}Y_{32}+X_{43}Y_{42}$

-

$X^T Y_{Val}$

$X_{41}Y_{41}$	$X_{41}Y_{42}$
$X_{42}Y_{41}$	$X_{42}Y_{42}$
$X_{43}Y_{41}$	$X_{43}Y_{42}$

Break up statistics into parts

Once:

    Compute parts for entire dataset

P times:

    Compute parts for validation set

    Derive training set parts

16 combinations of centering and scaling for **X** and **Y**

16 combinations of centering and scaling for **X** and **Y**

4 unique configurations for $\mathbf{X}^{\mathbf{T}}\mathbf{X}$

16 combinations of centering and scaling for **X** and **Y**

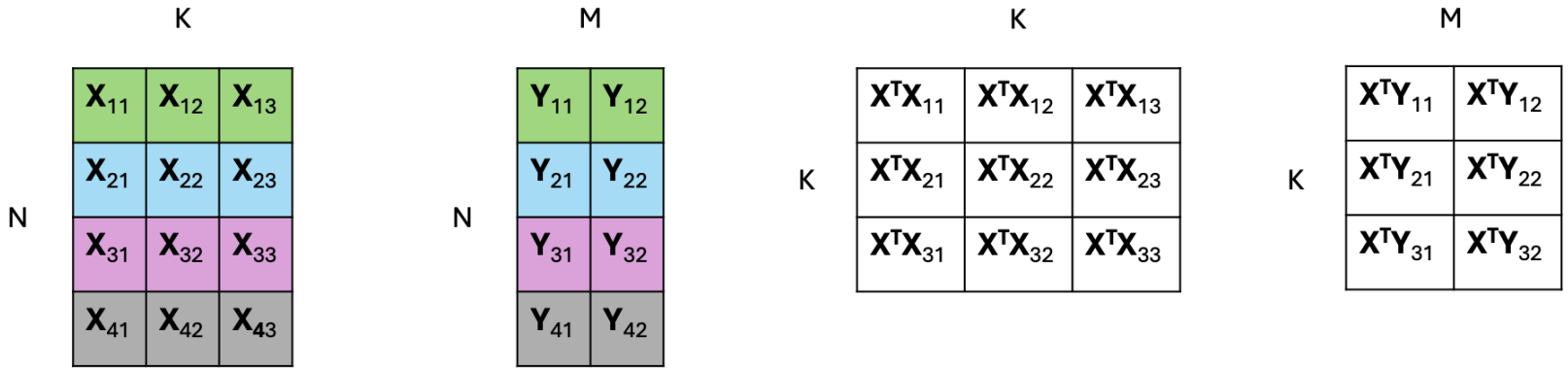
4 unique configurations for $\mathbf{X^TX}$
Only 8 unique configurations of $\mathbf{X^TY}$ (out of 16)

16 combinations of centering and scaling for **X** and **Y**

4 unique configurations for $\mathbf{X^TX}$

Only 8 unique configurations of $\mathbf{X^TY}$ (out of 16)

All improved from Θ(PNK(K+M)) to Θ(NK(K+M))



Algorithm 7 Fast Cross-Validation Algorithm with Centering and Scaling

Input: $\mathbf{X} \in \mathbb{R}^{N \times K}$, $\mathbf{Y} \in \mathbb{R}^{N \times M}$, $\mathcal{P}$ is a scalable partitioning of $R = \{1, \ldots, N\}$

$R \leftarrow \{1, \ldots, N\}$

Let $\mathcal{V}$ be the result of executing Algorithm 1 with $\mathcal{P}$ and R as input

$\mathrm{XTX} \leftarrow \mathbf{X^T X}$, $\mathrm{XTY} \leftarrow \mathbf{X^T Y}$, $\mu\mathrm{x} \leftarrow \overline{\mathbf{x}}$, $\mu\mathrm{y} \leftarrow \overline{\mathbf{y}}$

$\Sigma\mathrm{X} \leftarrow \sum_{n \in R} \mathbf{X}_n$, $\Sigma\mathrm{Y} \leftarrow \sum_{n \in R} \mathbf{Y}_n$, $\Sigma sq\mathrm{X} \leftarrow \sum_{n \in R} \left(\mathbf{X}_n^{\circ 2}\right)$, $\Sigma sq\mathrm{Y} \leftarrow \sum_{n \in R} \left(\mathbf{Y}_n^{\circ 2}\right)$

for each partition $p \in \{1, \ldots, P\}$ **do**

  $V \leftarrow \mathcal{V}[p]$

  $\mathrm{X}_V \leftarrow \mathbf{X}_V$, $\mathrm{Y}_V \leftarrow \mathbf{Y}_V$

  $\mathrm{XTX}_V \leftarrow \mathrm{X}_V^{\mathbf{T}} \mathrm{X}_V$, $\mathrm{XTY}_V \leftarrow \mathrm{X}_V^{\mathbf{T}} \mathrm{Y}_V$

  $\mathrm{XTX}_T \leftarrow \mathrm{XTX} - \mathrm{XTX}_V$, $\mathrm{XTY}_T \leftarrow \mathrm{XTY} - \mathrm{XTY}_V$ ▷ Obtain $\mathbf{X}_T^{\mathbf{T}} \mathbf{X}_T$ and $\mathbf{X}_T^{\mathbf{T}} \mathbf{Y}_T$

  $\mu\mathrm{x}_V \leftarrow \overline{\mathbf{x}_V}$, $\mu\mathrm{y}_V \leftarrow \overline{\mathbf{y}_V}$

  $N_V \leftarrow |V|$, $N_T \leftarrow N - N_V$

  $\mu\mathrm{x}_T \leftarrow \frac{N}{N_T} \mu\mathrm{x} - \frac{N_V}{N_T} \mu\mathrm{x}_V$ ▷ Obtain $\overline{\mathbf{x}_T}$

  $\mu\mathrm{y}_T \leftarrow \frac{N}{N_T} \mu\mathrm{y} - \frac{N_V}{N_T} \mu\mathrm{y}_V$ ▷ Obtain $\overline{\mathbf{y}_T}$

  $\mu\mathrm{xTx}_T \leftarrow N_T \left(\mu\mathrm{x}_T^{\mathbf{T}} \mu\mathrm{x}_T\right)$, $\mu\mathrm{xTy}_T \leftarrow N_T \left(\mu\mathrm{x}_T^{\mathbf{T}} \mu\mathrm{y}_T\right)$ ▷ Obtain $|T| \overline{\mathbf{x}_T^{\mathbf{T}}} \overline{\mathbf{x}_T}$ and $|T| \overline{\mathbf{x}_T^{\mathbf{T}}} \overline{\mathbf{y}_T}$

  $\mathrm{cXTX}_T \leftarrow \mathrm{XTX}_T - \mu\mathrm{xTx}_T$ ▷ Obtain $\mathbf{X}_T^{\mathbf{cT}} \mathbf{X}_T^{\mathbf{c}}$

  $\mathrm{cXTY}_T \leftarrow \mathrm{XTY}_T - \mu\mathrm{xTy}_T$ ▷ Obtain $\mathbf{X}_T^{\mathbf{cT}} \mathbf{Y}_T^{\mathbf{c}}$

  $\Sigma\mathrm{X}_V \leftarrow \sum_{n \in V} \mathrm{X}_n$, $\Sigma\mathrm{Y}_V \leftarrow \sum_{n \in V} \mathrm{Y}_n$

  $\Sigma\mathrm{X}_T \leftarrow \Sigma\mathrm{X} - \Sigma\mathrm{X}_V$, $\Sigma\mathrm{Y}_T \leftarrow \Sigma\mathrm{Y} - \Sigma\mathrm{Y}_V$ ▷ Obtain $\Sigma_{n \in T} \mathbf{X}_n$ and $\Sigma_{n \in T} \mathbf{Y}_n$

  $\Sigma sq\mathrm{X}_V \leftarrow \sum_{n \in V} \left(\mathbf{X}_n^{\circ 2}\right)$, $\Sigma sq\mathrm{Y}_V \leftarrow \sum_{n \in V} \left(\mathbf{Y}_n^{\circ 2}\right)$

  $\Sigma sq\mathrm{X}_T \leftarrow \Sigma sq\mathrm{X} - \Sigma sq\mathrm{X}_V$ ▷ Obtain $\Sigma_{n \in T} \left(\mathbf{X}_n^{\circ 2}\right)$

  $\Sigma sq\mathrm{Y}_T \leftarrow \Sigma sq\mathrm{Y} - \Sigma sq\mathrm{Y}_V$ ▷ Obtain $\Sigma_{n \in T} \left(\mathbf{Y}_n^{\circ 2}\right)$

  $\sigma\mathrm{x}_T \leftarrow \left(\frac{1}{N_T - 1} \left(-2\mu\mathrm{x}_T \odot \Sigma\mathrm{X}_T + N_T \mu\mathrm{x}_T^{\circ 2} + \Sigma sq\mathrm{X}_T\right)\right)^{\circ \frac{1}{2}}$ ▷ Obtain $\widehat{\mathbf{x}_T}$

  $\sigma\mathrm{y}_T \leftarrow \left(\frac{1}{N_T - 1} \left(-2\mu\mathrm{y}_T \odot \Sigma\mathrm{Y}_T + N_T \mu\mathrm{y}_T^{\circ 2} + \Sigma sq\mathrm{Y}_T\right)\right)^{\circ \frac{1}{2}}$ ▷ Obtain $\widehat{\mathbf{y}_T}$

  Replace with 1 any entry in $\sigma\mathrm{x}_T$ and $\sigma\mathrm{y}_T$ that is 0.

  $\sigma\mathrm{xTx}_T \leftarrow \sigma\mathrm{x}_T^{\mathbf{T}} \sigma\mathrm{x}_T$, $\sigma\mathrm{xTy}_T \leftarrow \sigma\mathrm{x}_T^{\mathbf{T}} \sigma\mathrm{y}_T$ ▷ Obtain $\widehat{\mathbf{x}_T^{\mathbf{T}}} \widehat{\mathbf{x}_T}$ and $\widehat{\mathbf{x}_T^{\mathbf{T}}} \widehat{\mathbf{y}_T}$

  $\mathrm{csXTX}_T \leftarrow \mathrm{cXTX}_T \oslash \sigma\mathrm{xTx}_T$ ▷ Obtain $\mathbf{X}_T^{\mathbf{csT}} \mathbf{X}_T^{\mathbf{cs}}$

  $\mathrm{csXTY}_T \leftarrow \mathrm{cXTY}_T \oslash \sigma\mathrm{xTy}_T$ ▷ Obtain $\mathbf{X}_T^{\mathbf{csT}} \mathbf{Y}_T^{\mathbf{csT}}$

end for

Does it really matter?

Does it really matter?

Demo time!

Contributions

Faster cross-validation for $\mathbf{X^TX}$ and $\mathbf{X^TY}$

Solved for any combination of centering and scaling

Software implementing the algorithm

pip install cvmatrix

Software combining the algorithm with PLS

pip install ikpls

Article