# Linear Regression



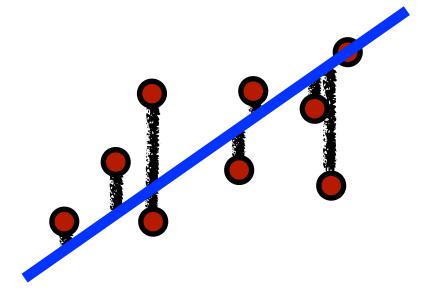


# Regression

Goal: Learn a mapping from observations (features) to

**Example:** Height, Gender, Weight  $\rightarrow$  Shoe Size

- Audio features  $\rightarrow$  Song year
- Processes, memory  $\rightarrow$  Power consumption
- Historical financials  $\rightarrow$  Future stock price
- Many more



- continuous labels given a training set (supervised learning)

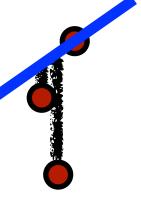
We assume a *linear* mapping between features and label:



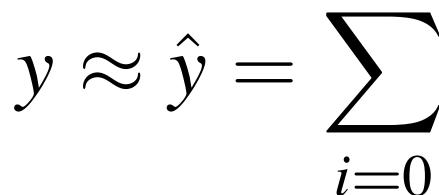
**Example:** Predicting shoe size from height, gender, and weight

For each observation we have a feature vector,  $\mathbf{x}$ , and label, y  $\mathbf{x}^{\top} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}$ 

- $y \approx w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$



We can augment the feature vector to incorporate offset:

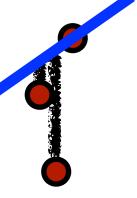




**Example:** Predicting shoe size from height, gender, and weight

 $\mathbf{x}^{\top} = \begin{bmatrix} 1 & x_1 & x_2 & x_3 \end{bmatrix}$ 

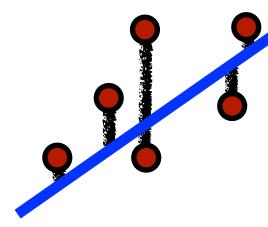
We can then rewrite this linear mapping as scalar product: 3  $y \approx \hat{y} = \sum w_i x_i = \mathbf{w}^{\top} \mathbf{x}$ 



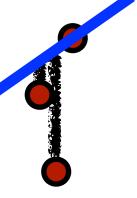
# Why a Linear Mapping?

### **Often works well in practice**

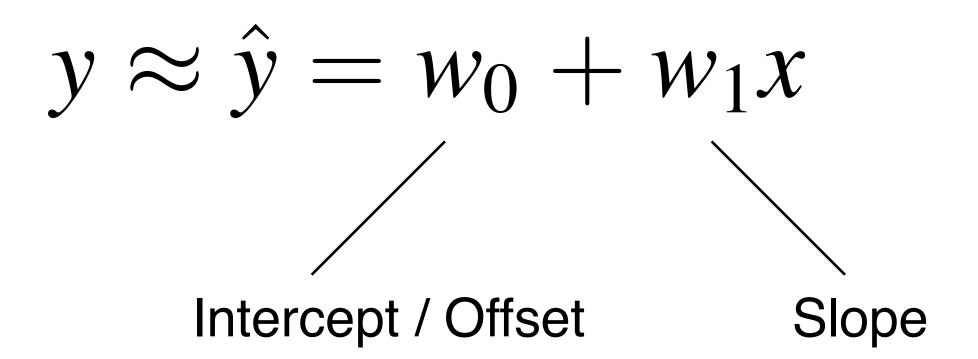
### **Can introduce complexity via feature extraction**



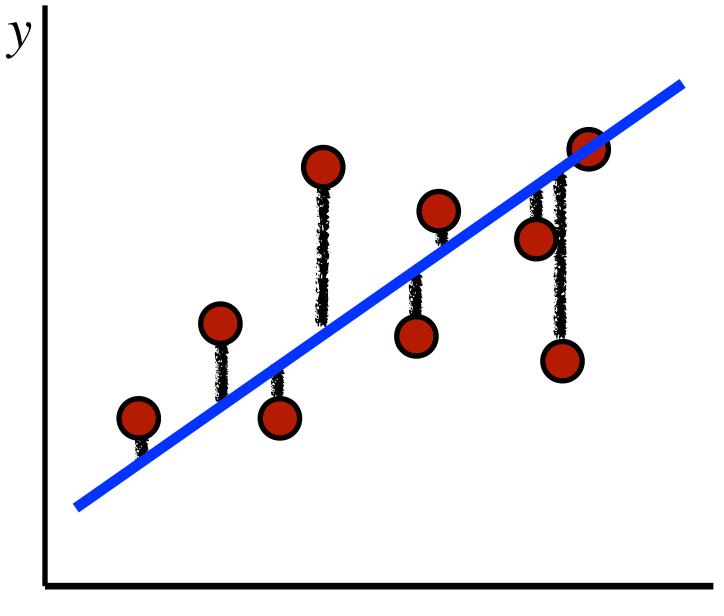
### Simple



### **Goal**: find the line of best fit x coordinate: features y coordinate: labels



### 1D Example



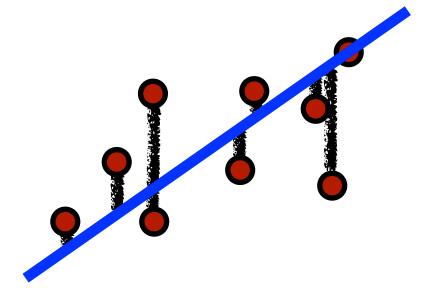
 $\mathcal{X}$ 

# Evaluating Predictions

- Can measure 'closeness' between label and prediction • Shoe size: better to be off by one size than 5 sizes • Song year prediction: better to be off by a year than by 20 years

What is an appropriate evaluation metric or 'loss' function?

- Absolute loss:  $|y \hat{y}|$
- Squared loss:  $(y \hat{y})^2$  Has nice mathematical properties



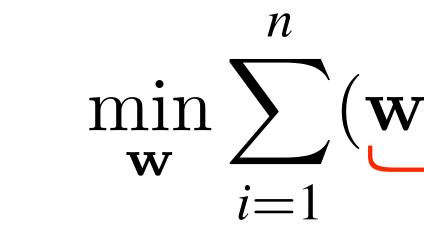
# How Can We Learn Model (w)?

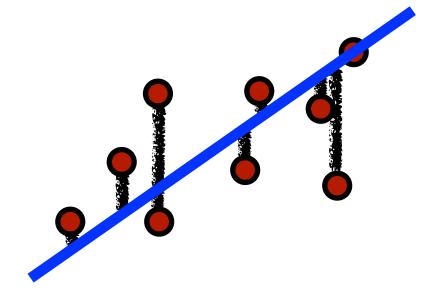
Assume we have *n* training points, where  $\mathbf{x}^{(i)}$  denotes the *i*th point

Recall two earlier points:

- Linear assumption:  $\hat{y} = \mathbf{w}^\top \mathbf{x}$
- We use squared loss:  $(y \hat{y})^2$

Idea: Find  $\mathbf{w}$  that minimizes squared loss over training points:





### **x** 2

$$\mathbf{x}^{\top}\mathbf{x}^{(i)} - y^{(i)})^2$$

$$\hat{y}^{(i)}$$

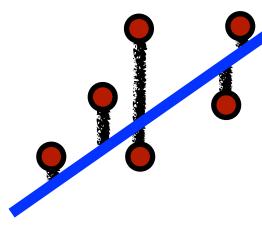
# • $\mathbf{X} \in \mathbb{R}^{n \times d}$ : matrix storing points • $\mathbf{y} \in \mathbb{R}^n$ : real-valued labels

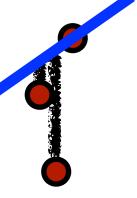
•  $\mathbf{\hat{y}} \in \mathbb{R}^{n}$ : predicted labels, where  $\mathbf{\hat{y}} = \mathbf{X}\mathbf{w}$ •  $\mathbf{w} \in \mathbb{R}^d$ : regression parameters / model to learn

Equivalent  $\min_{\mathbf{w}} \sum_{i=1}^{\infty} (\mathbf{w}^{\top} \mathbf{x}^{(i)} - y^{(i)})^2$  by definition of Euclidean norm

- Given *n* training points with *d* features, we define:

Least Squares Regression: Learn mapping (w) from features to labels that minimizes residual sum of squares:  $\min ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2$ 



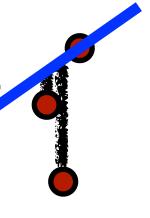


Find solution by setting derivative to zero  
1D: 
$$f(w) = ||w\mathbf{x} - \mathbf{y}||_2^2 = \sum_{i=1}^n (wx^{(i)} - y^{(i)})^2$$
  
 $\frac{df}{dw}(w) = 2\sum_{i=1}^n x^{(i)}(wx^{(i)} - y^{(i)}) = 0 \iff w\mathbf{x}^\top \mathbf{x} - \mathbf{x}^\top \mathbf{y} = 0$   
 $\underbrace{w\mathbf{x}^\top \mathbf{x} - \mathbf{x}^\top \mathbf{y}}_{w\mathbf{x}^\top \mathbf{x} - \mathbf{x}^\top \mathbf{y}} \iff w = (\mathbf{x}^\top \mathbf{x})^{-1} \mathbf{x}^\top \mathbf{y}$ 

# $\mathbf{W}$

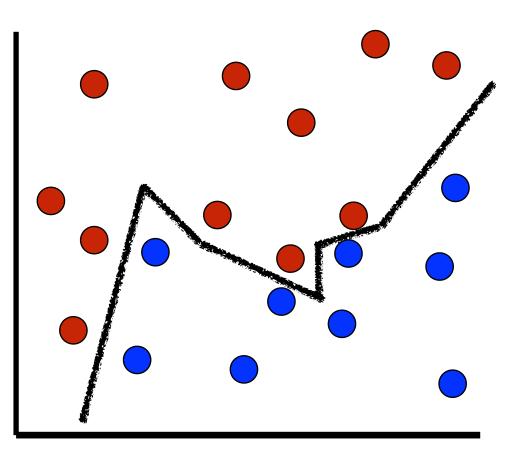
Closed form solution:  $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$  (if inverse exists)

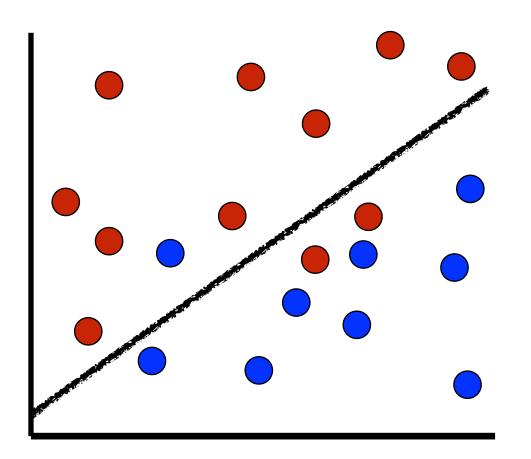
Least Squares Regression: Learn mapping (w) from features to labels that minimizes residual sum of squares:  $\min ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2$ 



# Overfitting and Generalization

- We want good predictions on new data, i.e., 'generalization'
- Least squares regression minimizes training error, and could overfit • Simpler models are more likely to generalize (Occam's razor)
- Can we change the problem to penalize for model complexity? Intuitively, models with smaller weights are simpler

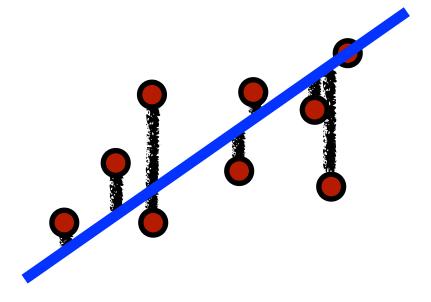




•  $\mathbf{X} \in \mathbb{R}^{n \times d}$ : matrix storing points •  $\mathbf{y} \in \mathbb{R}^n$ : real-valued labels •  $\hat{\mathbf{y}} \in \mathbb{R}^n$ : predicted labels, where  $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$ 

Closed-form solution:  $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X} + \lambda \mathbf{I}_d)^{-1}\mathbf{X}^{\top}\mathbf{y}$ 

- Given *n* training points with *d* features, we define:



- $\mathbf{w} \in \mathbb{R}^d$ : regression parameters / model to learn

**Ridge Regression:** Learn mapping (w) that minimizes residual sum of squares along with a regularization term: Training Error Model Complexity  $\min_{\mathbf{w}} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \lambda ||\mathbf{w}||_2^2$ 

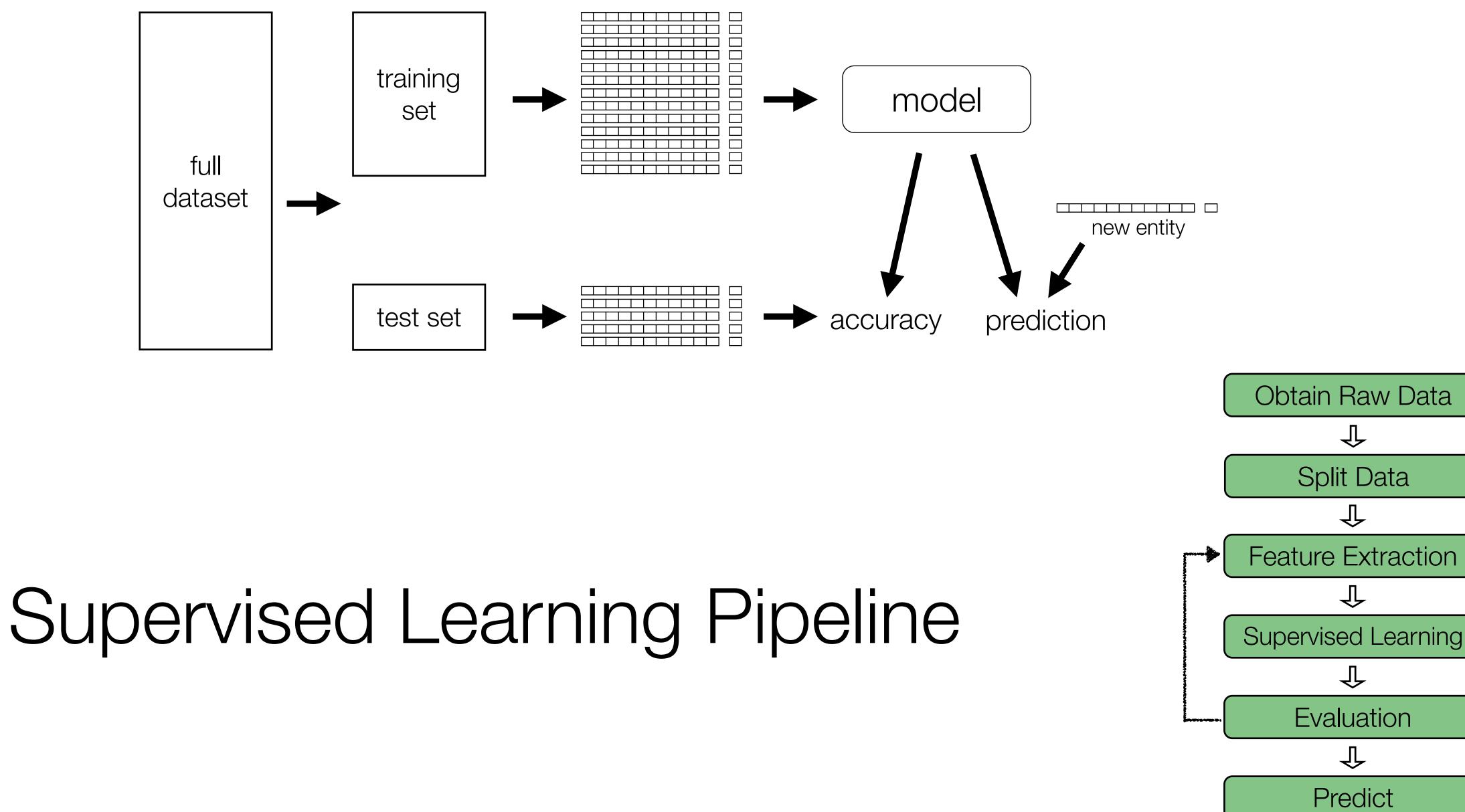
free parameter trades off between training error and model complexity



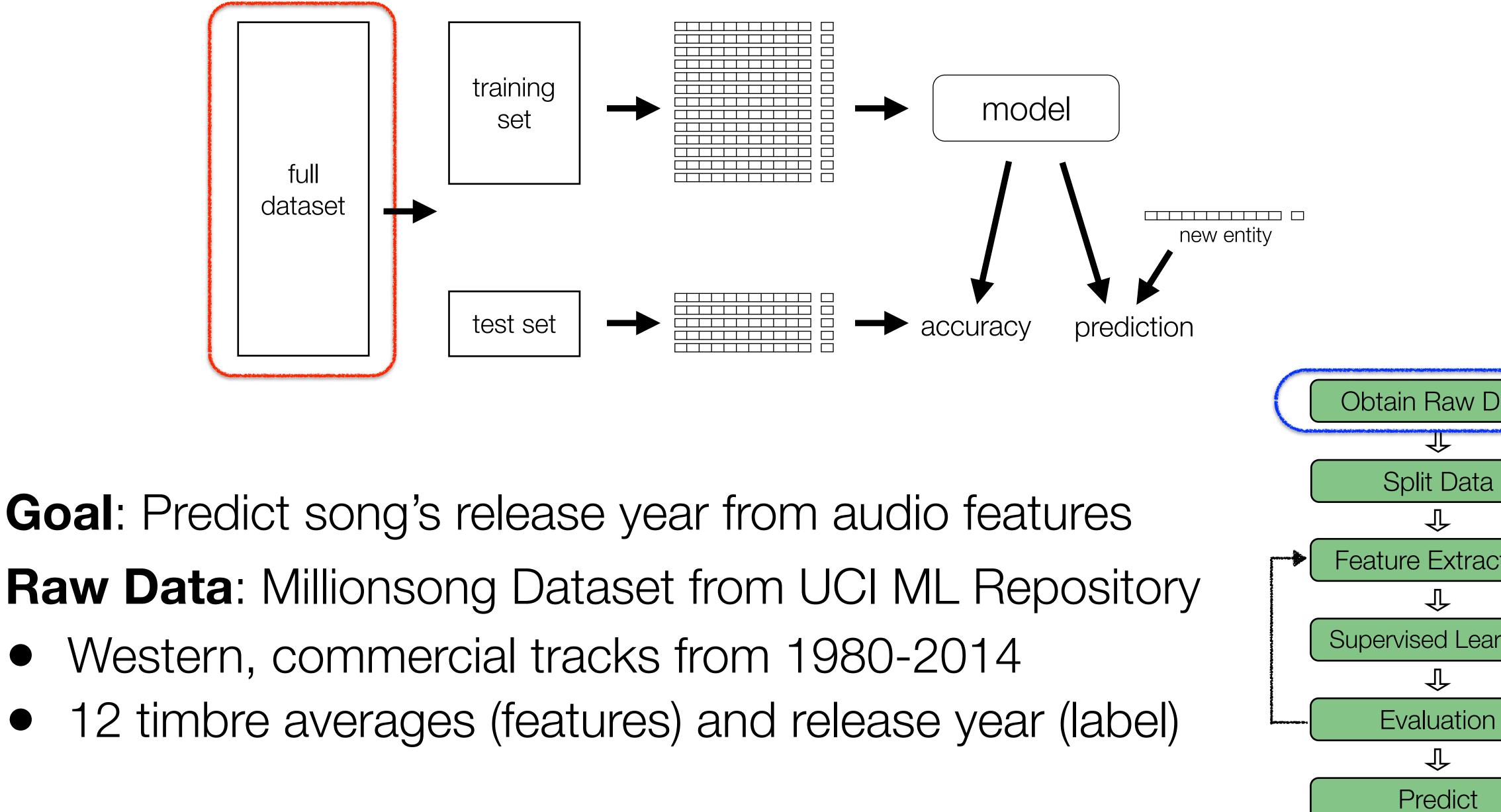
# Millionsong Regression Pipeline



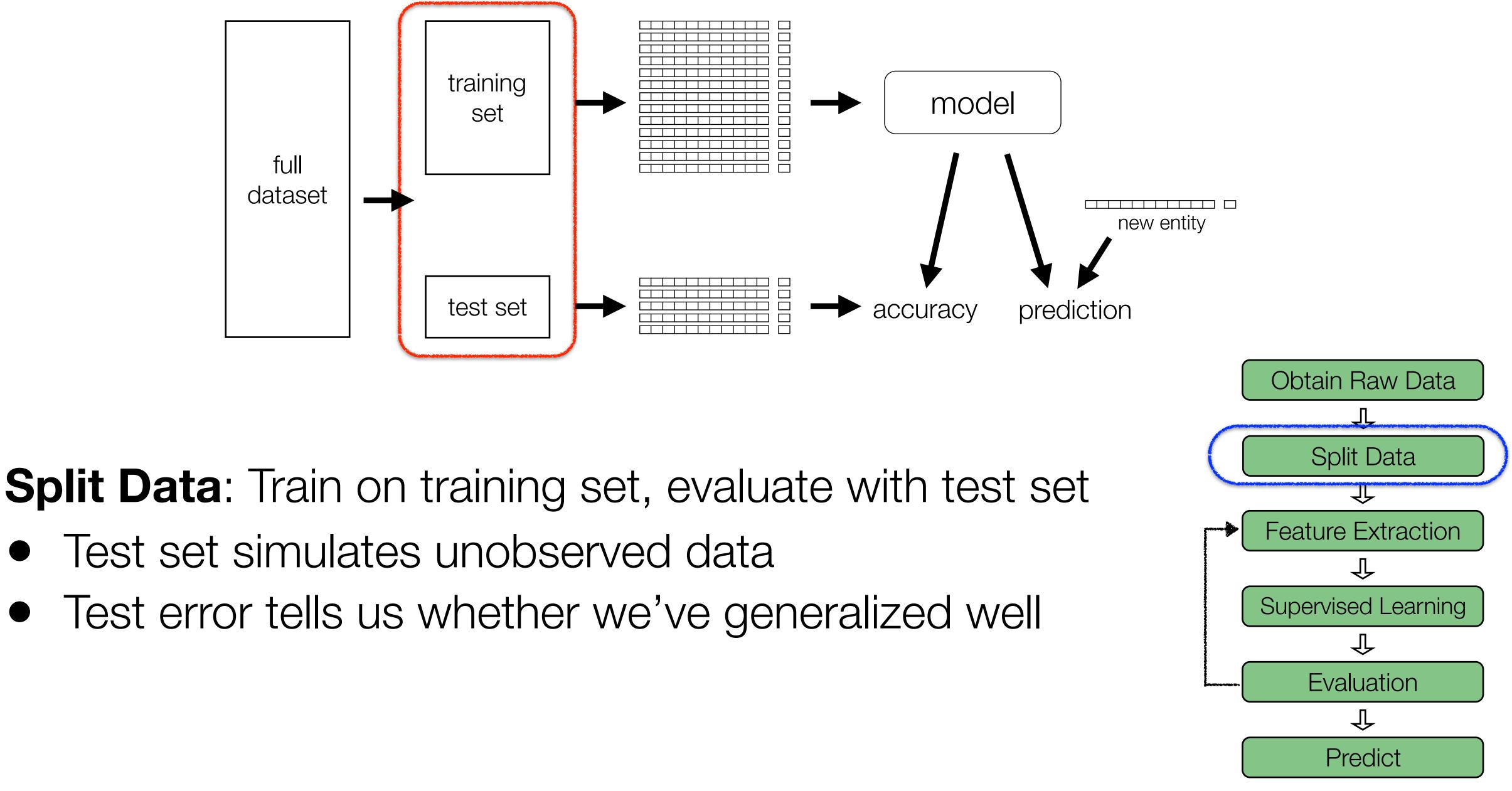




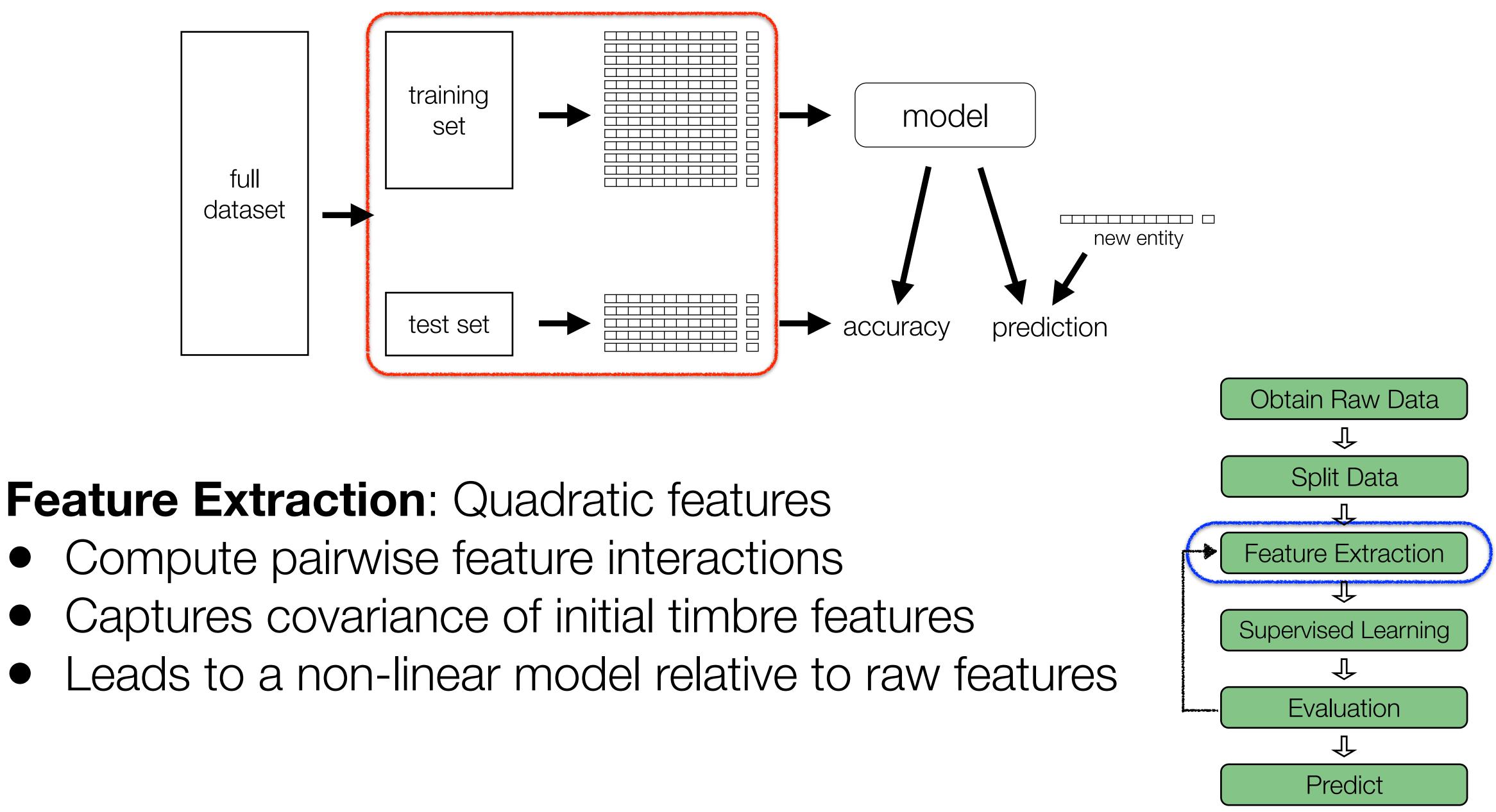
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- Test set simulates unobserved data



$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top \implies \Phi(z)$$
$$\mathbf{z} = \begin{bmatrix} z_1 & z_2 \end{bmatrix}^\top \implies \Phi(z)$$

More succinctly:  

$$\Phi'(\mathbf{x}) = \begin{bmatrix} x_1^2 & \sqrt{2}x_1x_2 & x_2^2 \end{bmatrix}^{-1}$$

Equivalent inner products:

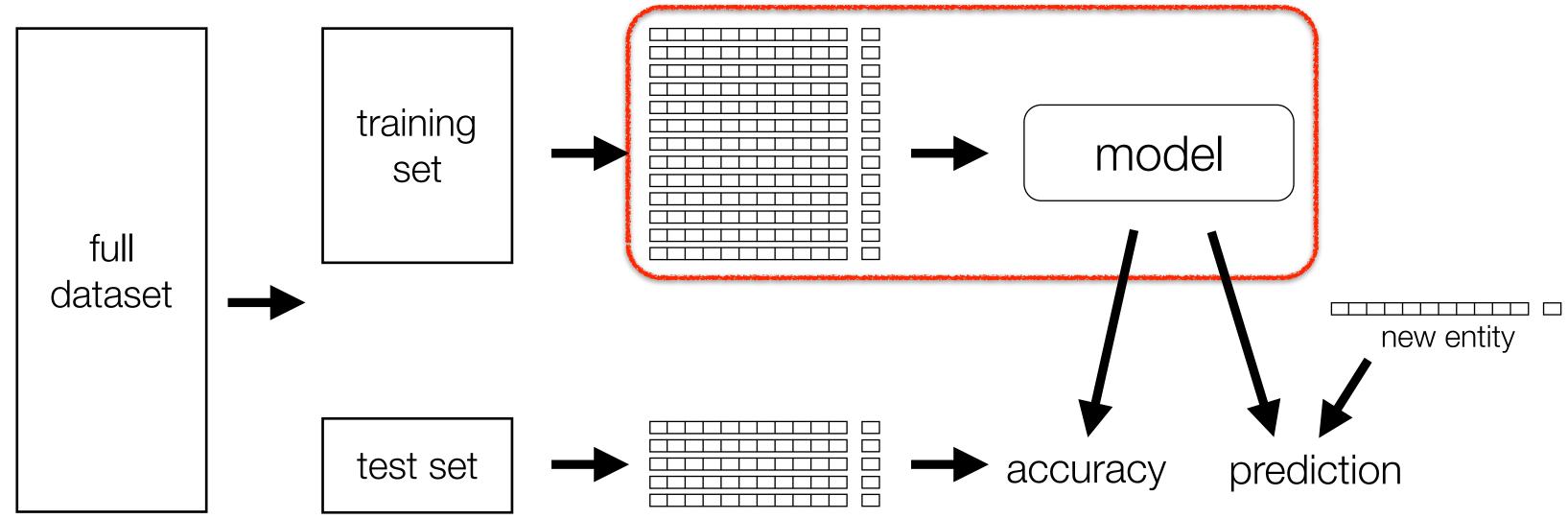
$$\Phi(\mathbf{x})^{\top} \Phi(\mathbf{z}) = \sum x_1^2 z_1^2 + 2x$$

Given 2 dimensional data, quadratic features are:

 $(\mathbf{x}) = \begin{bmatrix} x_1^2 & x_1 x_2 & x_2 x_1 & x_2^2 \end{bmatrix}^{\top}$  $(\mathbf{z}) = \begin{bmatrix} z_1^2 & z_1 z_2 & z_2 z_1 & z_2^2 \end{bmatrix}^{\top}$ 

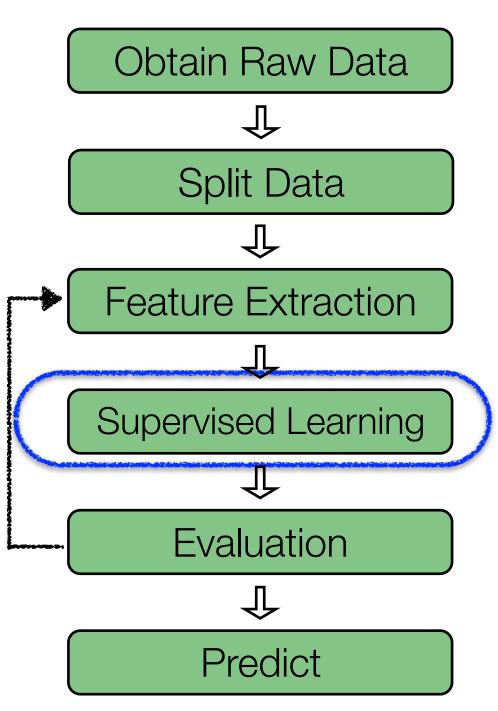
 $\top \quad \Phi'(\mathbf{z}) = \begin{bmatrix} z_1^2 & \sqrt{2}z_1z_2 & z_2^2 \end{bmatrix}^{\top}$ 

 $x_1 x_2 z_1 z_2 + x_2^2 z_2^2 = \Phi'(\mathbf{x}) \Phi'(\mathbf{z})$ 



### Supervised Learning: Least Squares Regression • Learn a mapping from entities to continuous

- labels given a training set
- Audio features → Song year

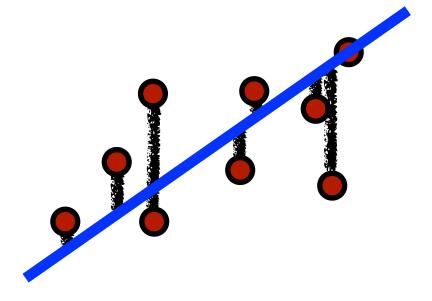


•  $\mathbf{X} \in \mathbb{R}^{n \times d}$ : matrix storing points •  $\mathbf{y} \in \mathbb{R}^n$ : real-valued labels •  $\mathbf{\hat{y}} \in \mathbb{R}^n$ : predicted labels, where  $\mathbf{\hat{y}} = \mathbf{X}\mathbf{w}$ 

W

Closed-form solution:

- Given *n* training points with *d* features, we define:



- $\mathbf{w} \in \mathbb{R}^d$ : regression parameters / model to learn

**Ridge Regression:** Learn mapping (w) that minimizes residual sum of squares along with a regularization term: Training Error Model Complexity

 $\min_{\mathbf{W}} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \lambda ||\mathbf{w}||_2^2$ 

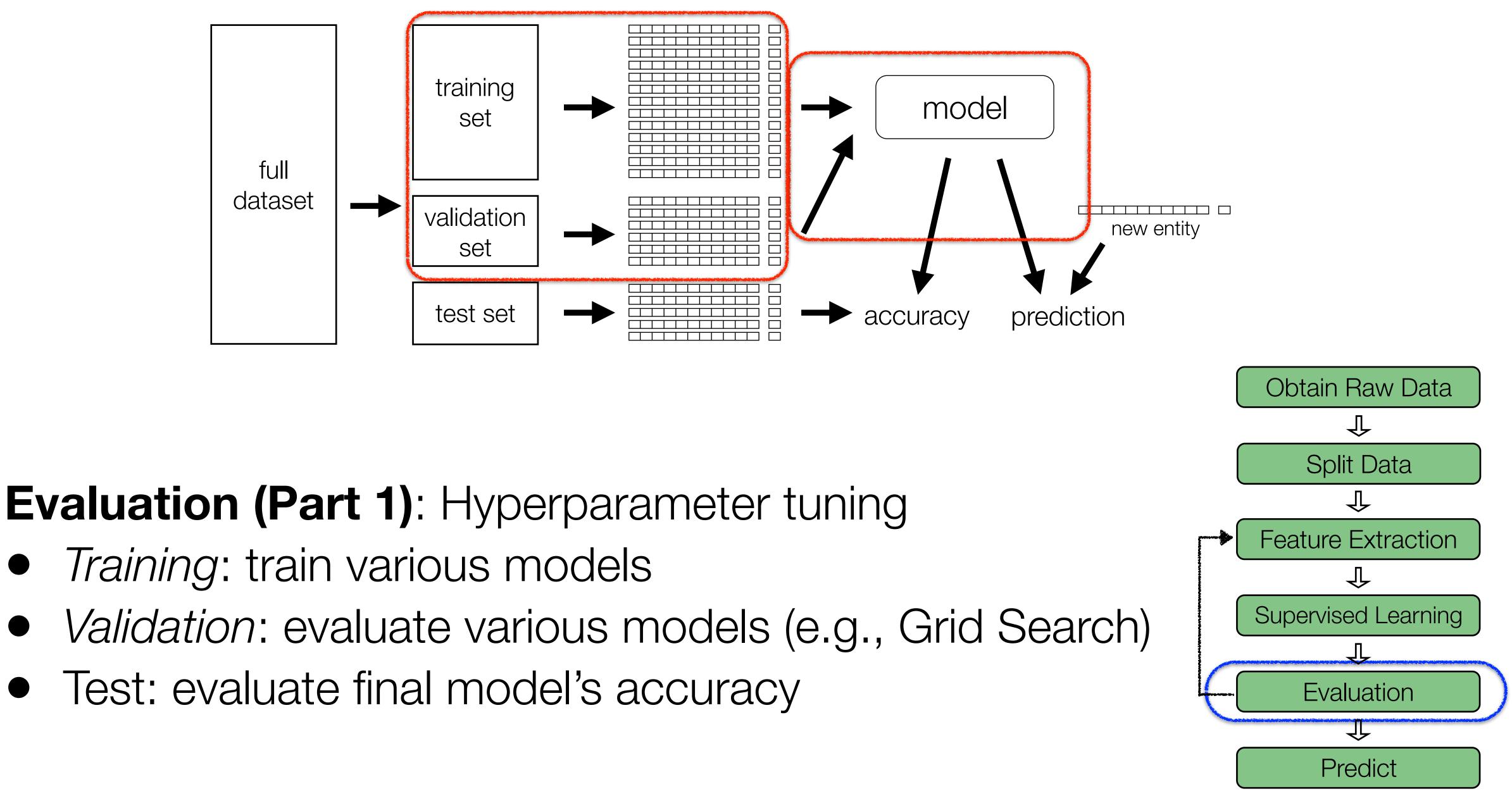
$$\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X} + \lambda\mathbf{I}_d)^{-1}\mathbf{X}^{\top}\mathbf{y}$$



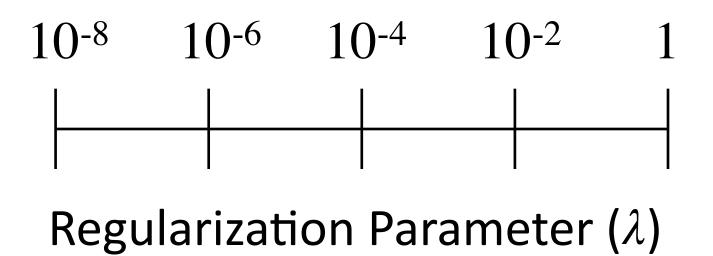
- free parameter trades off between training ... error and model complexity
- How do we choose a good value for this free parameter? Most methods have free parameters / 'hyperparameters' to tune
- First thought: Search over multiple values, evaluate each on test set • But, goal of test set is to simulate unobserved data
- We may overfit if we use it to choose hyperparameters

### **Ridge Regression**: Learn mapping (w) that minimizes residual sum of squares along with a regularization term: Training Error Model Complexity $\min_{\mathbf{w}} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \lambda ||\mathbf{w}||_2^2$

### Second thought: Create another hold out dataset for this search

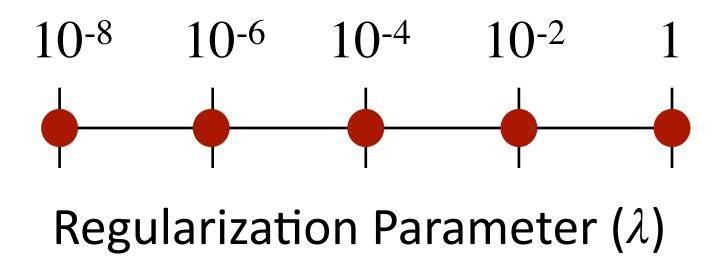


- *Training*: train various models
- Test: evaluate final model's accuracy

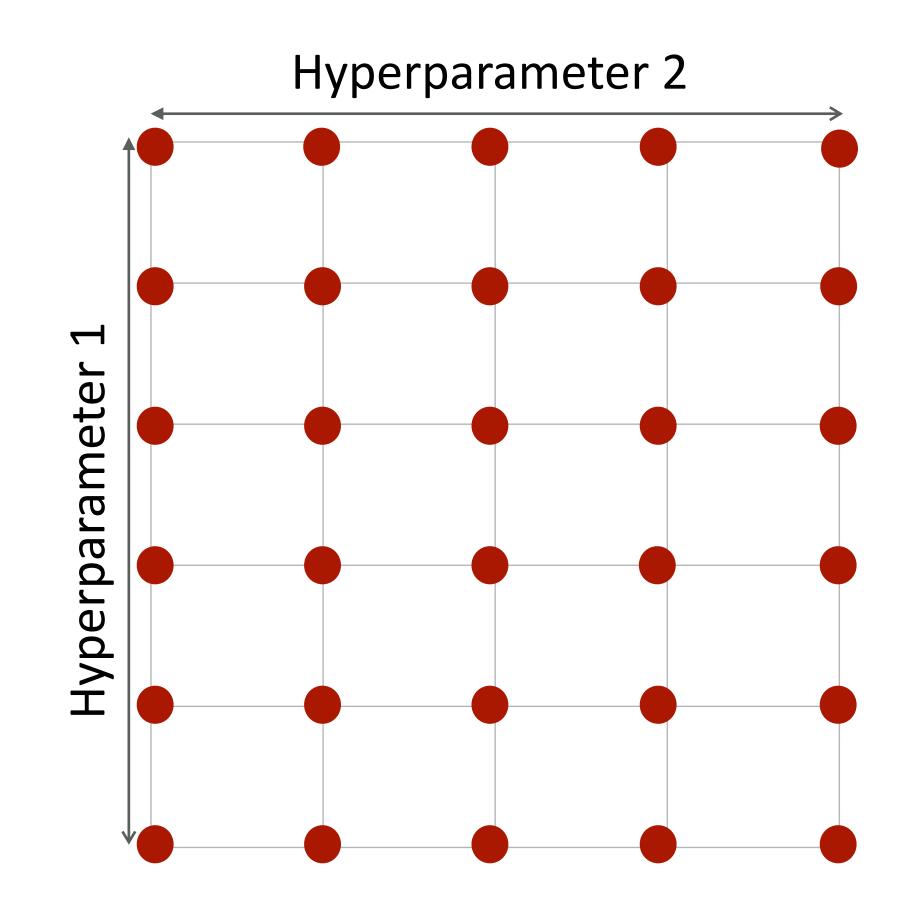


- Define and discretize search space (linear or log scale)
- Evaluate points via validation error

Grid Search: Exhaustively search through hyperparameter space



- Define and discretize search space (linear or log scale)
- Evaluate points via validation error



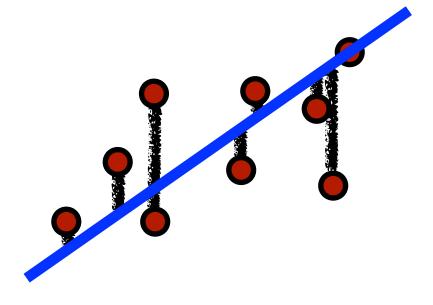
Grid Search: Exhaustively search through hyperparameter space

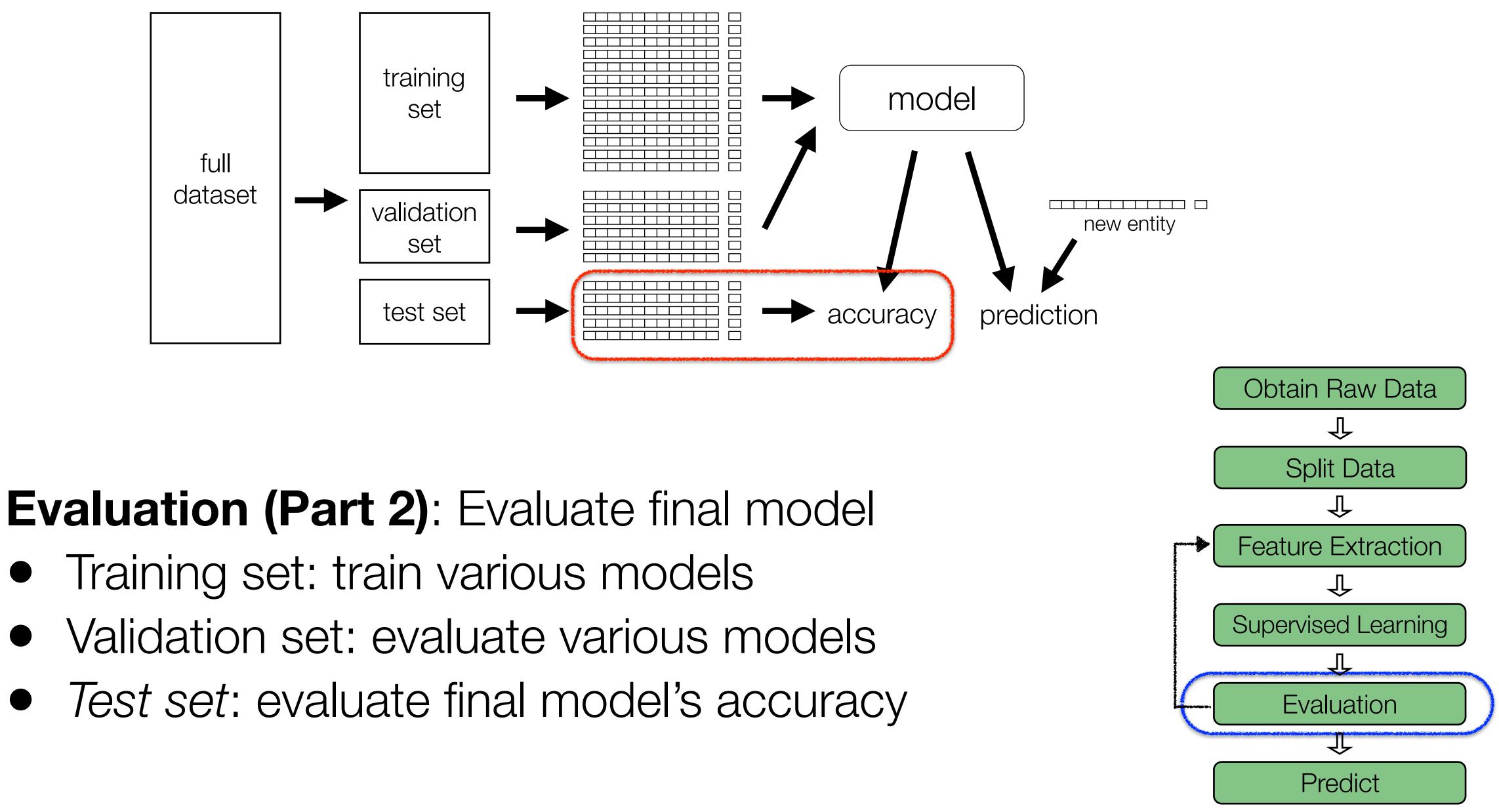
# Evaluating Predictions

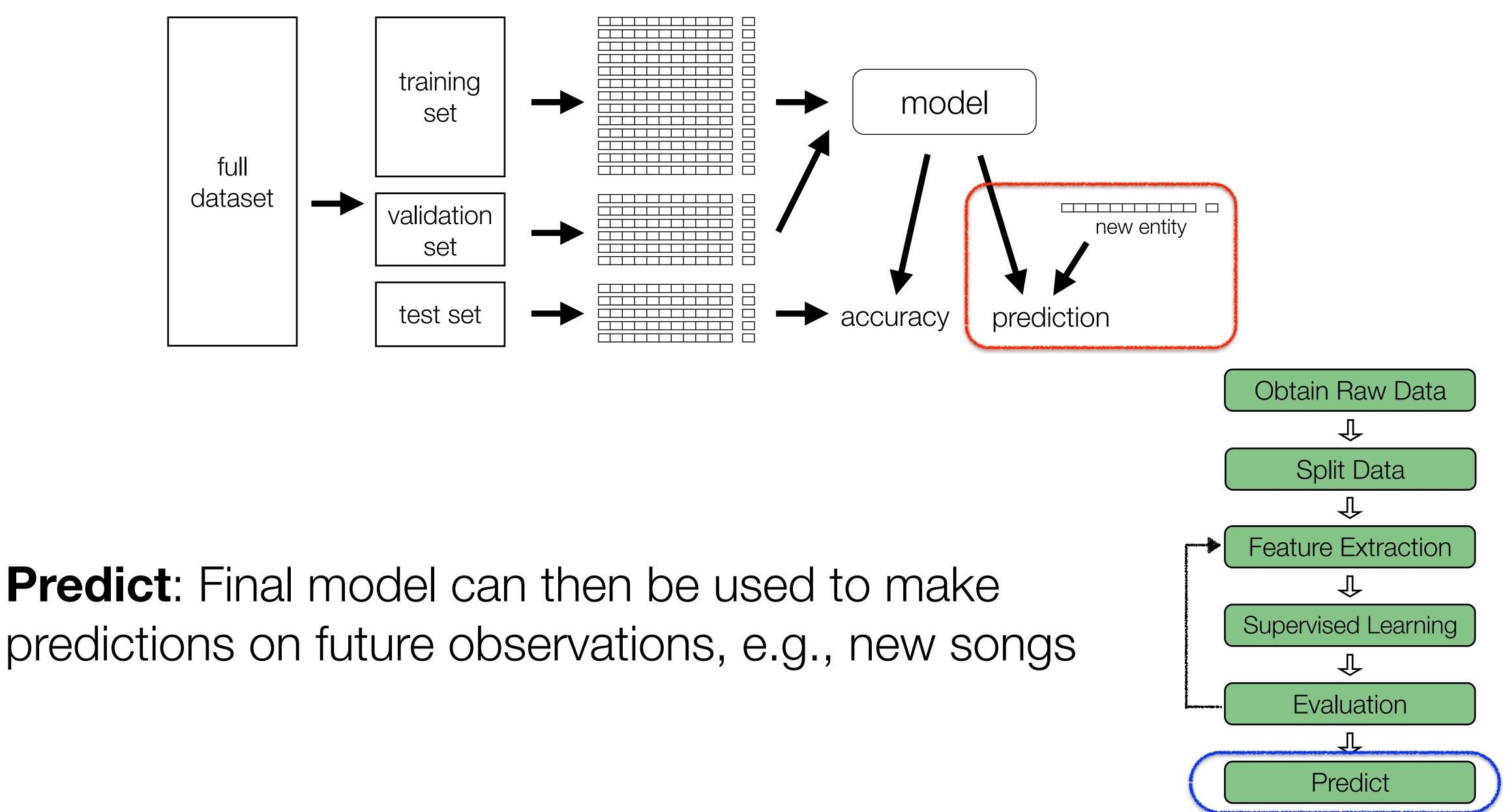
- How can we compare labels and predictions for *n* validation points?
- Least squares optimization involves squared loss,  $(y \hat{y})^2$ , so it seems reasonable to use mean squared error (**MSE**):

MSE = 
$$\frac{1}{n} \sum_{i=1}^{n} (\hat{y}^{(i)} - y^{(i)})^2$$

- But MSE's unit of measurement is square of quantity being measured, e.g., "squared years" for song prediction
- More natural to use root-mean-square error (**RMSE**), i.e.,  $\sqrt{\text{MSE}}$





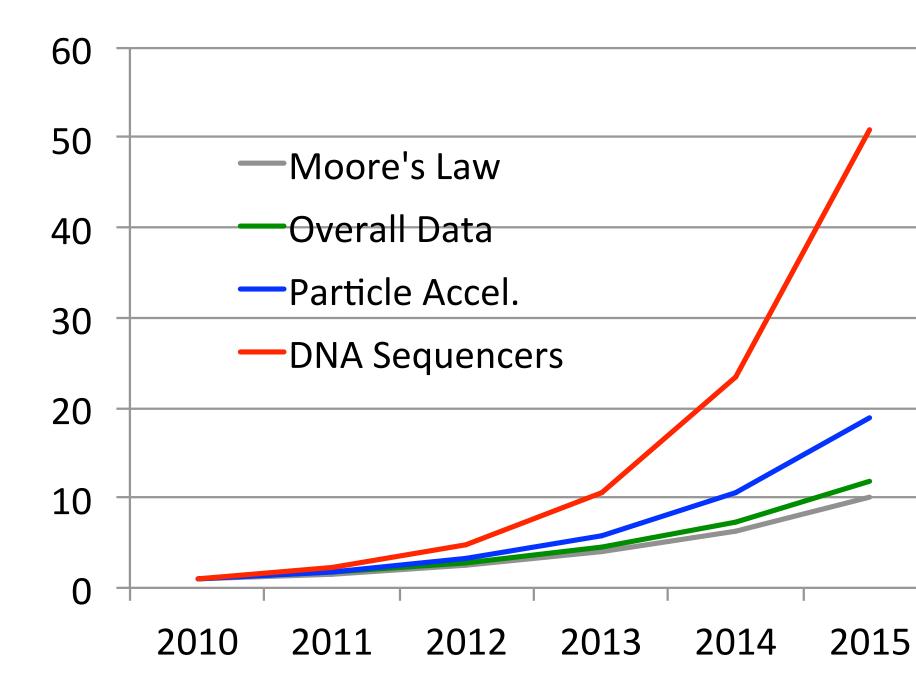


# Distributed ML: Computation and Storage



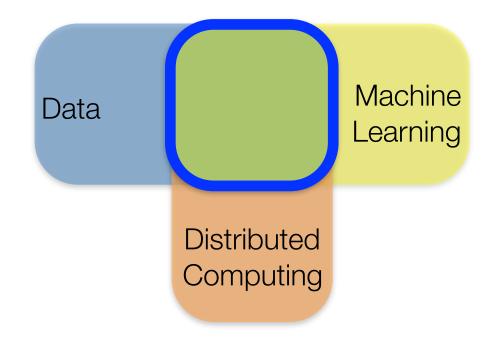


# Challenge: Scalability



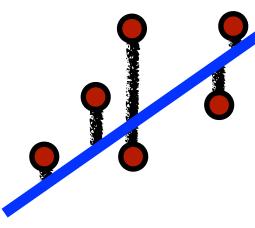
Classic ML techniques are not always suitable for modern datasets

Data Grows Faster than Moore's Law [IDC report, Kathy Yelick, LBNL]



# min

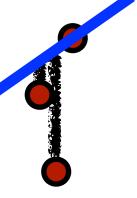
- How do we solve this computationally? Computational profile similar for Ridge Regression



Least Squares Regression: Learn mapping (w) from features to labels that minimizes residual sum of squares:

$$|{f X}{f w} - {f y}||_2^2$$

Closed form solution:  $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$  (if inverse exists)



# Computing Closed Form Solution

Computational bottlenecks:

- Matrix multiply of  $\mathbf{X}^{\top}\mathbf{X}$ : O(*nd*<sup>2</sup>) operations • Matrix inverse:  $O(d^3)$  operations

Other methods (Cholesky, QR, SVD) have same complexity

 $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

### Consider number of arithmetic operations $(+, -, \times, /)$

# Storage Requirements

**Storage**:  $O(nd + d^2)$  floats

Consider storing values as floats (8 bytes)

Storage bottlenecks:

- $\mathbf{X}^{\top}\mathbf{X}$  and its inverse:  $O(d^2)$  floats
- $\mathbf{X}$  : O(nd) floats

 $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

# Big *n* and Small *d*

**Storage**:  $O(nd + d^2)$  floats

single machine

Can distribute storage and computation! • Store data points (rows of  $\mathbf{X}$ ) across machines • Compute  $\mathbf{X}^{\top}\mathbf{X}$  as a sum of outer products

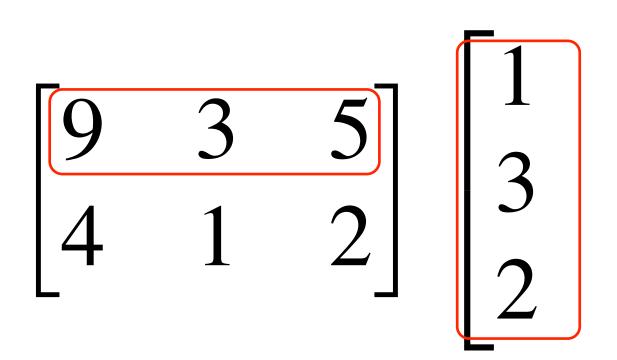
 $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

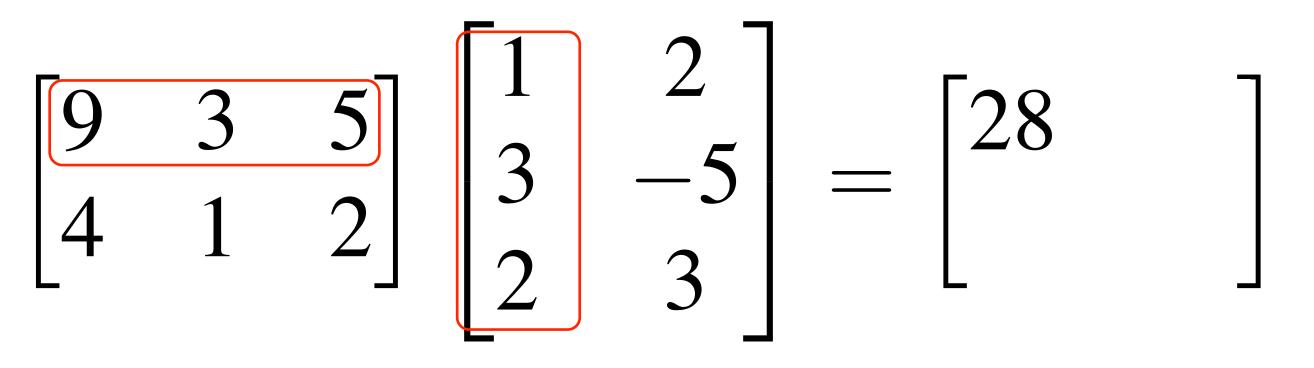
### Assume $O(d^3)$ computation and $O(d^2)$ storage feasible on

### Storing X and computing $\mathbf{X}^{\top}\mathbf{X}$ are the bottlenecks

# Matrix Multiplication via Inner Products

Each entry of output matrix is result of inner product of inputs matrices

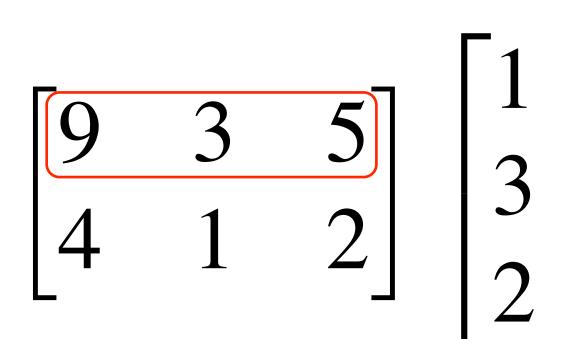


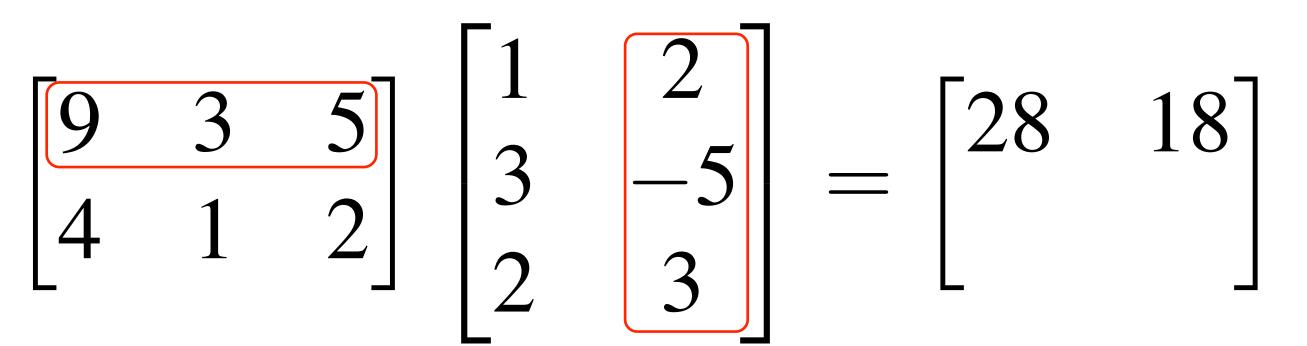


 $9 \times 1 + 3 \times 3 + 5 \times 2 = 28$ 

# Matrix Multiplication via Inner Products

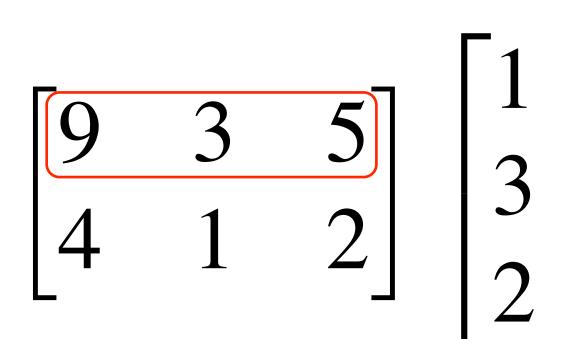
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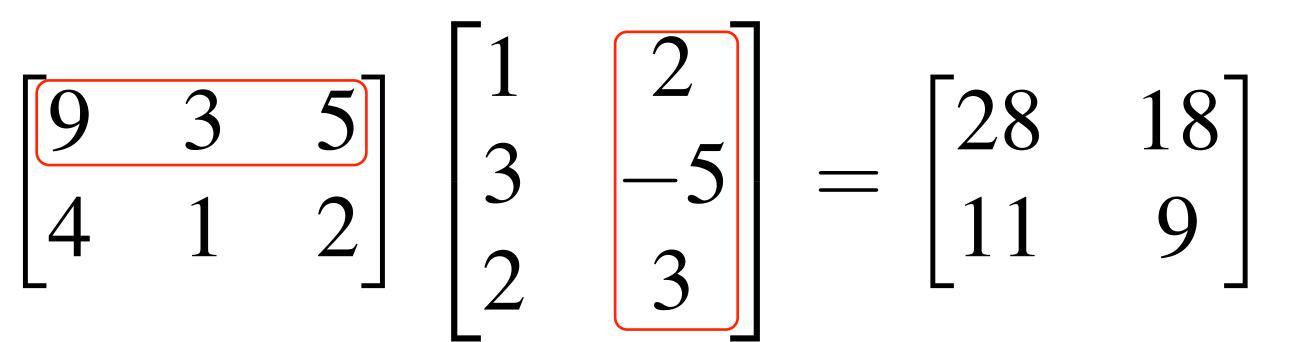


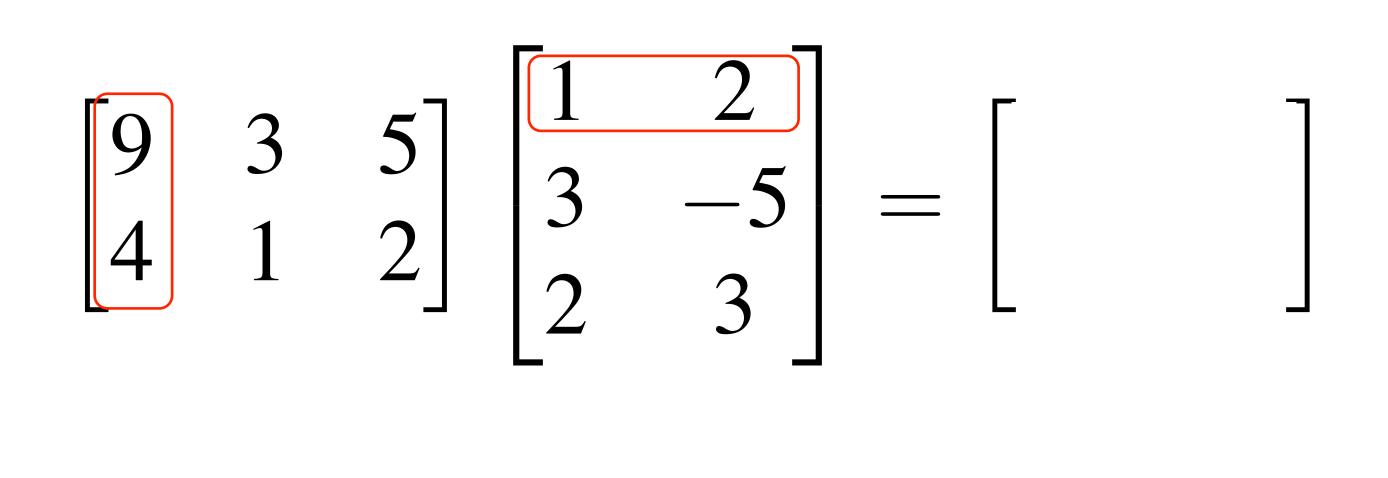


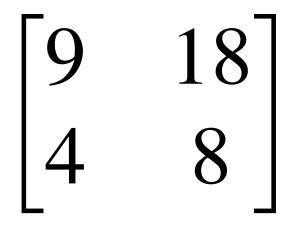
# Matrix Multiplication via Inner Products

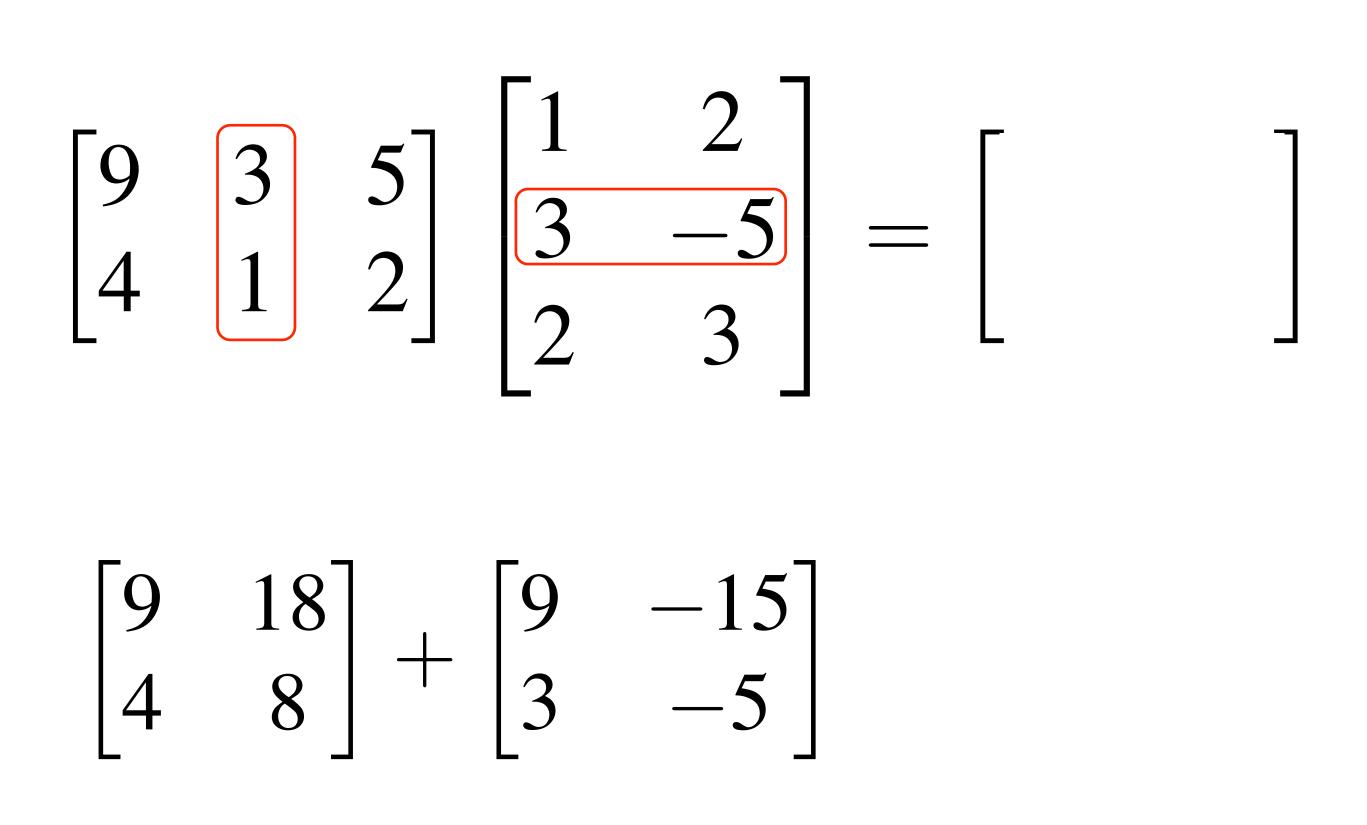
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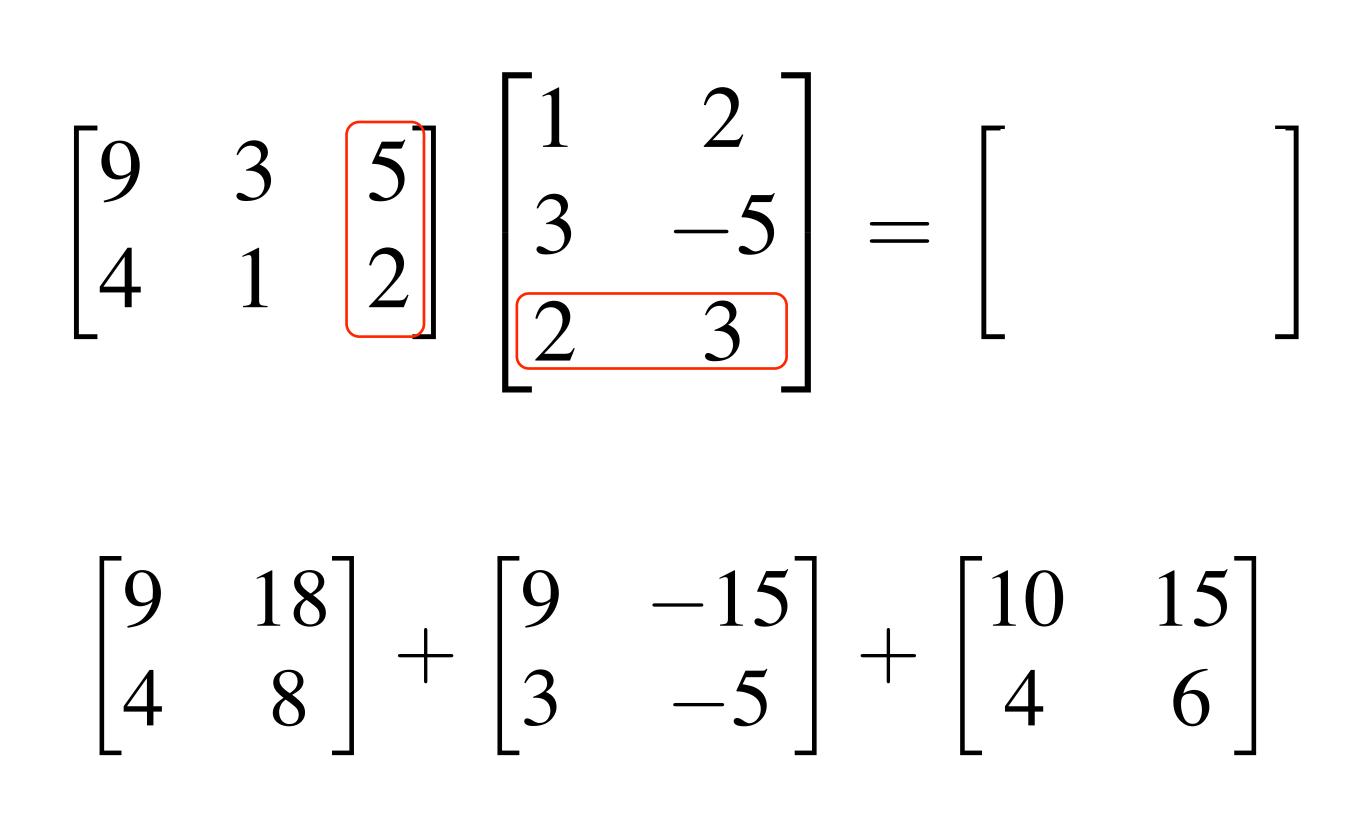


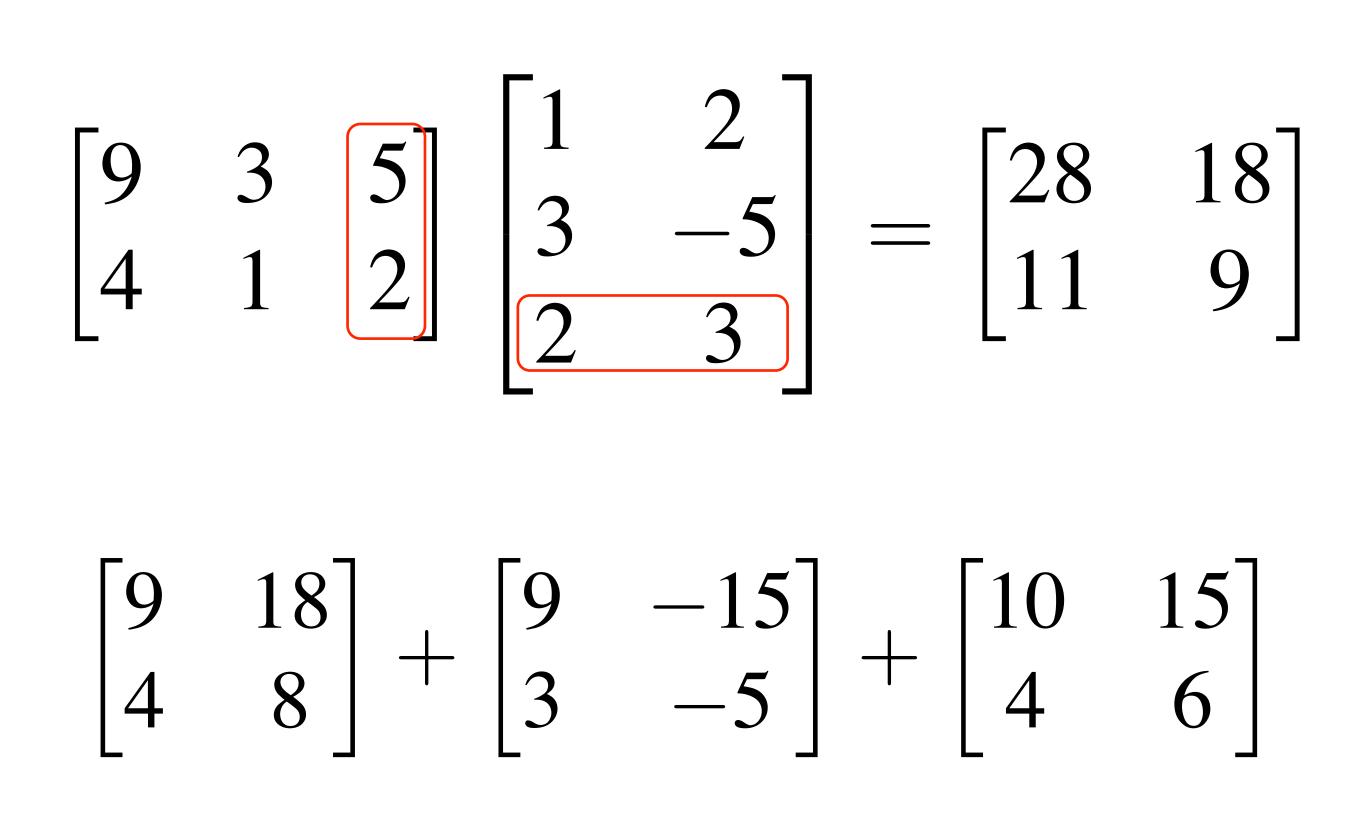


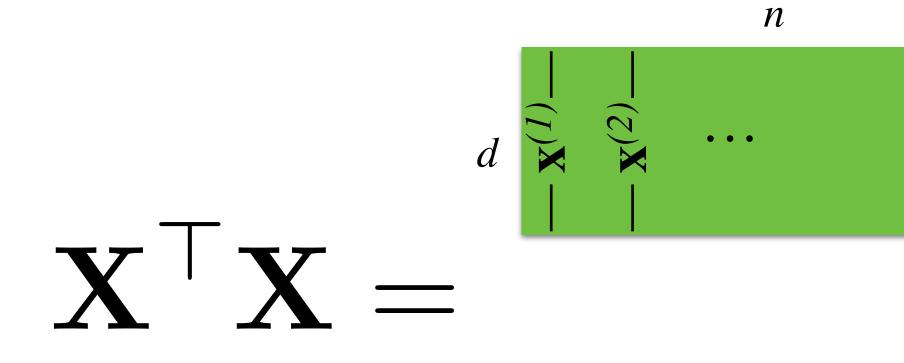




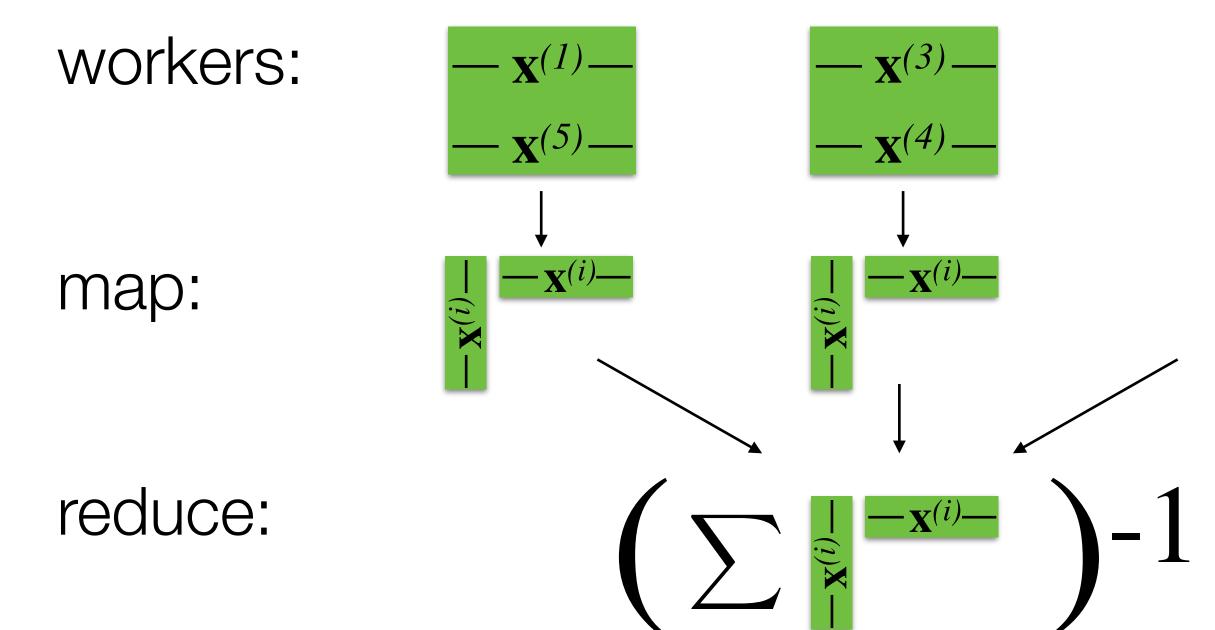


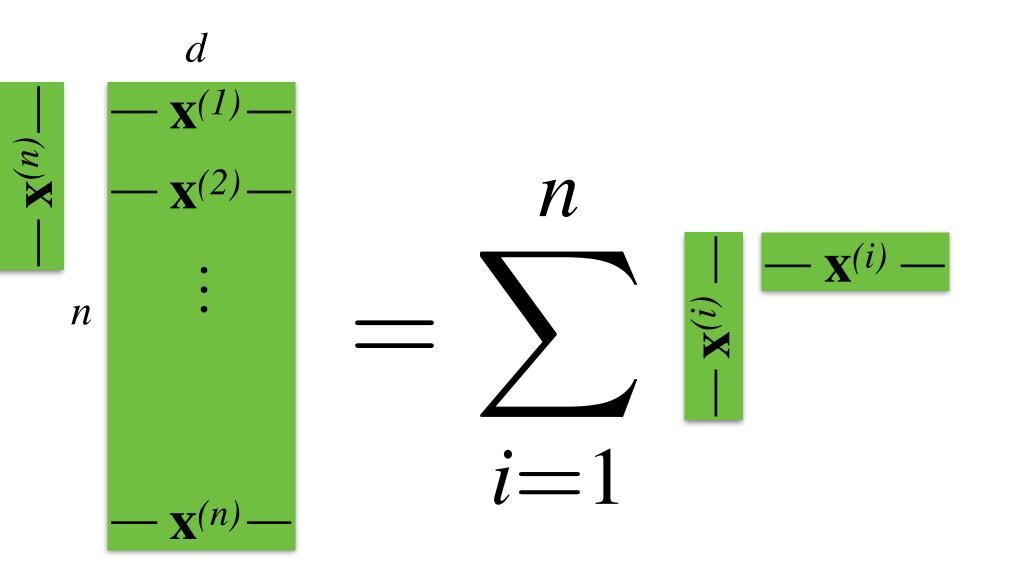


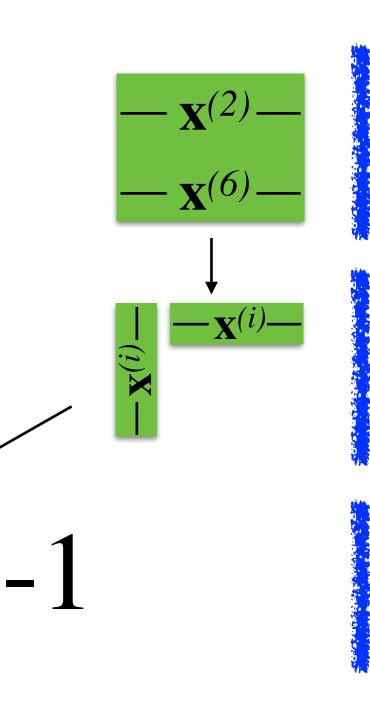




#### Example: n = 6; 3 workers







O(*nd*) Distributed Storage

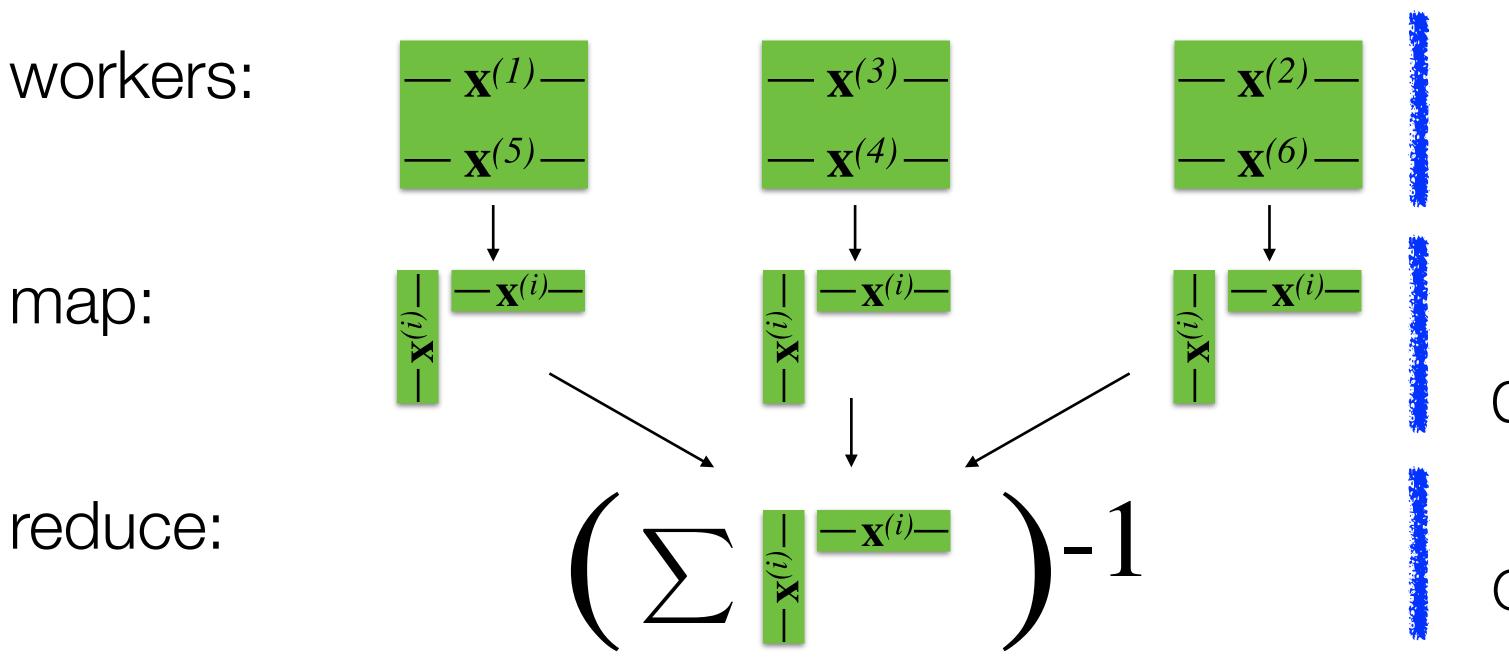
 $O(nd^2)$ Distributed Computation

 $O(d^2)$  Local Storage

 $O(d^3)$  Local  $O(d^2)$  Local Computation

Storage

## trainData.map(computeOuterProduct) .reduce(sumAndInvert)



O(*nd*) Distributed Storage

 $O(nd^2)$ Distributed Computation

 $O(d^2)$  Local Storage

 $O(d^3)$  Local  $O(d^2)$  Local Computation

Storage



# Distributed ML: Computation and Storage, Part II





## Big *n* and Small *d*

**Storage**:  $O(nd + d^2)$  floats

single machine

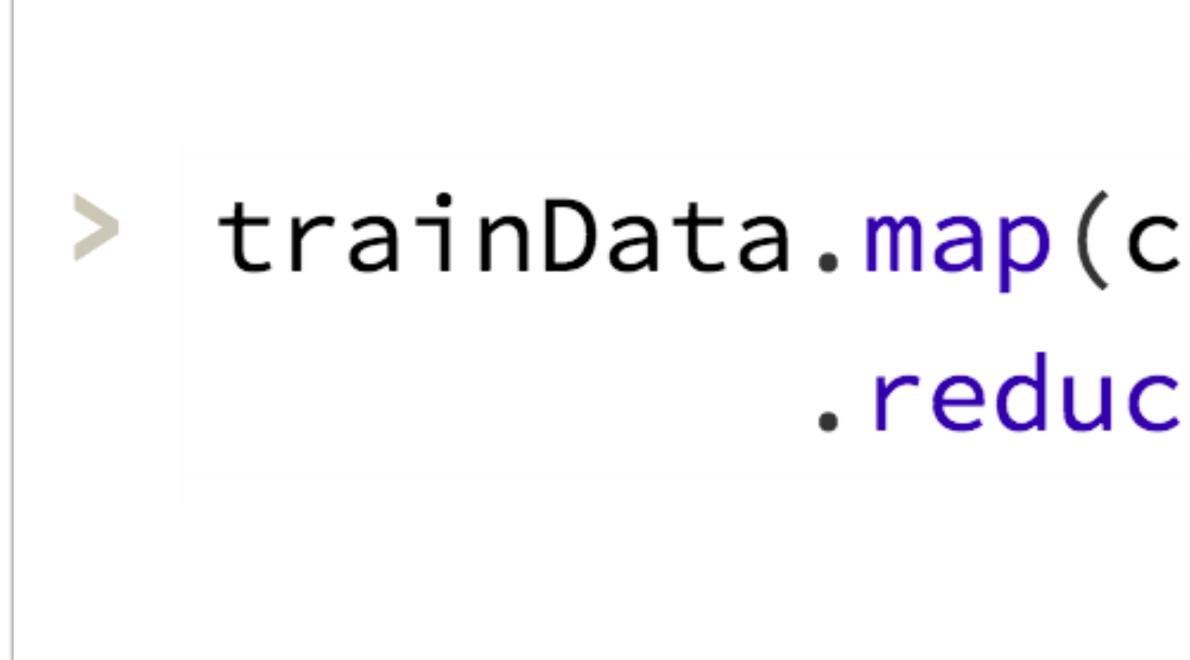
Can distribute storage and computation! • Store data points (rows of  $\mathbf{X}$ ) across machines • Compute  $\mathbf{X}^{\top}\mathbf{X}$  as a sum of outer products

 $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

### Assume $O(d^3)$ computation and $O(d^2)$ storage feasible on

## Big *n* and Small *d*

**Storage**:  $O(nd + d^2)$  floats



 $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

# trainData.map(computeOuterProduct) .reduce(sumAndInvert)

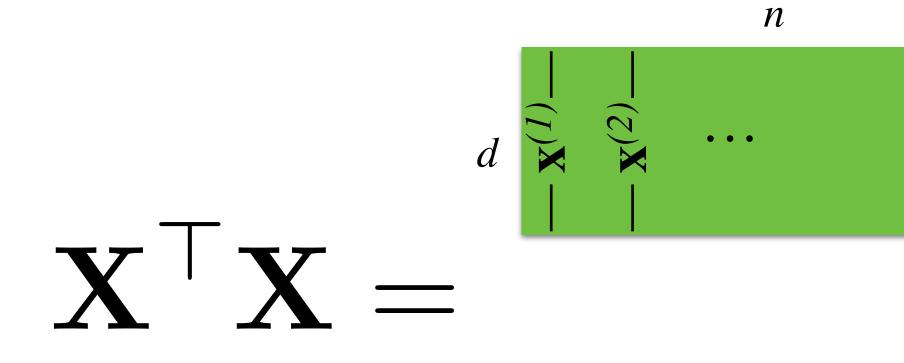


**Storage**:  $O(nd + d^2)$  floats

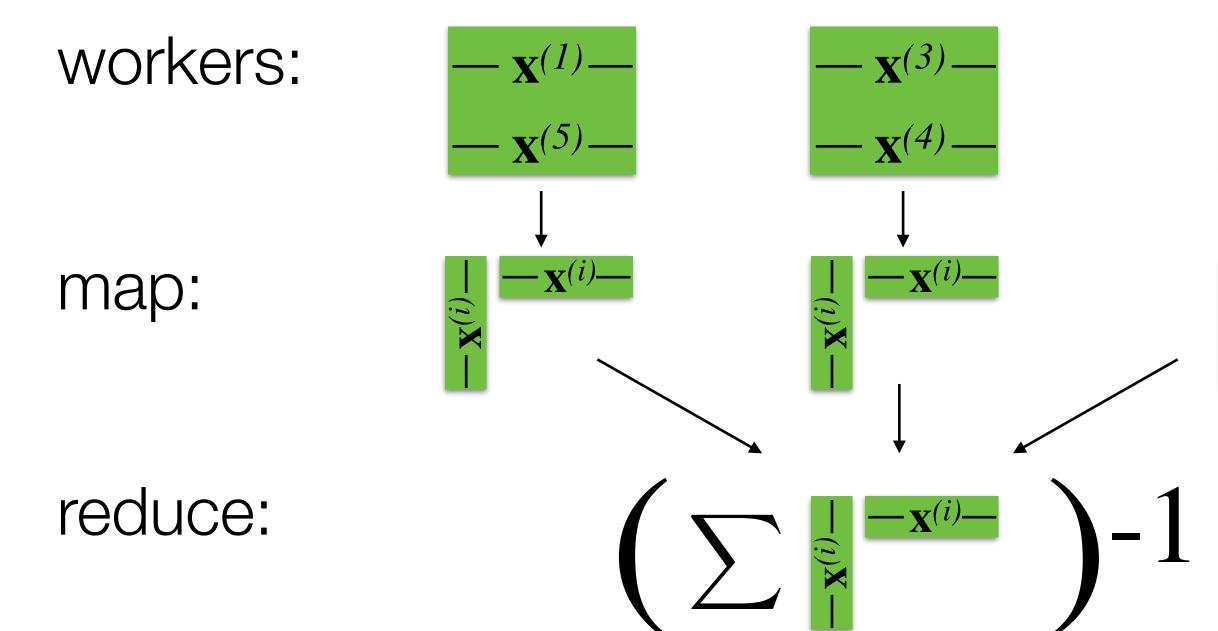
• Can't easily distribute!

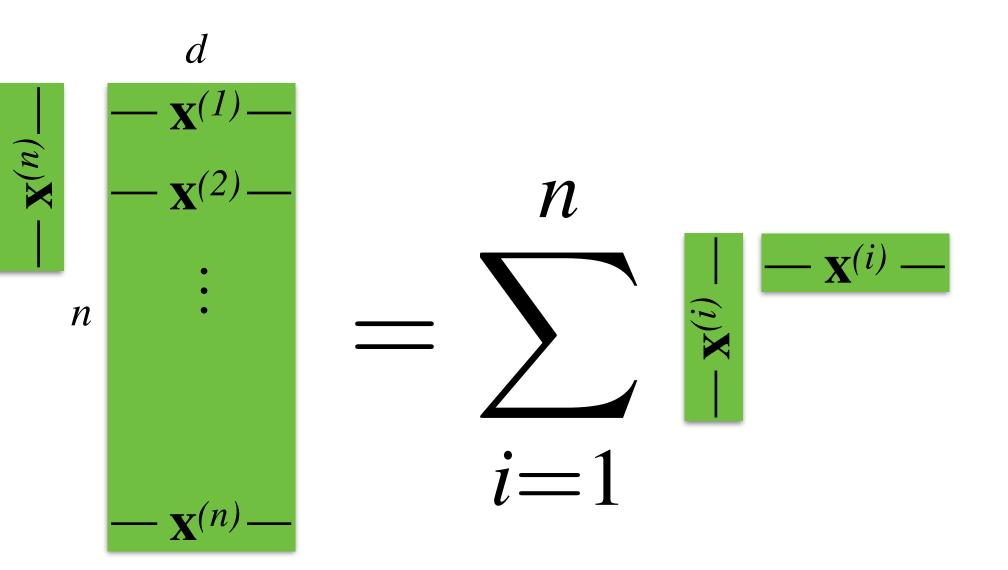
Big *n* and Big *d*  $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

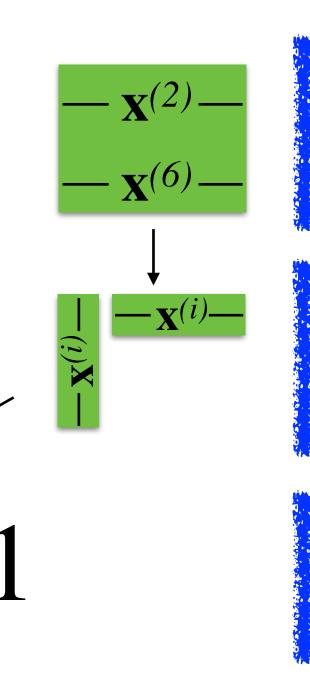
### As before, storing X and computing $\mathbf{X}^{\top}\mathbf{X}$ are bottlenecks Now, storing and operating on $\mathbf{X}^{\top}\mathbf{X}$ is also a bottleneck



#### Example: n = 6; 3 workers







#### O(*nd*) Distributed Storage

 $O(nd^2)$ <br/>Distributed<br/>Computation $O(d^2)$  Local<br/>Storage $O(d^3)$  Local<br/>Computation $O(d^2)$  Local<br/>Storage

**Storage**:  $O(nd + d^2)$  floats

• Can't easily distribute!

1st Rule of thumb Computation and storage should be linear (in n, d)

Big *n* and Big *d*  $\mathbf{w} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$ **Computation**:  $O(nd^2 + d^3)$  operations

### As before, storing X and computing $\mathbf{X}^{\top}\mathbf{X}$ are bottlenecks Now, storing and operating on $\mathbf{X}^{\top}\mathbf{X}$ is also a bottleneck

# Big *n* and Big *d*

### We need methods that are linear in time and space

### One idea: Exploit sparsity

• Explicit sparsity can provide orders of magnitude storage and computational gains

### Sparse data is prevalent

- Text processing: bag-of-words, n-grams
- Collaborative filtering: ratings matrix
- Graphs: adjacency matrix
- Categorical features: one-hot-encoding
- Genomics: SNPs, variant calling

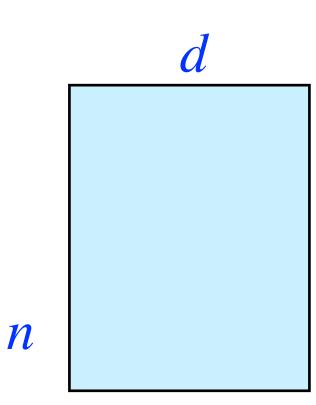
dense : 1. 0. 0. 0. 0. 0. 3.  
sparse : 
$$\begin{cases} size : 7 \\ indices : 0 & 6 \\ values : 1. 3. \end{cases}$$

## Big *n* and Big *d*

We need methods that are linear in time and space

### One idea: **Exploit sparsity**

- computational gains



• Explicit sparsity can provide orders of magnitude storage and

 Latent sparsity assumption can be used to reduce dimension, e.g., PCA, low-rank approximation (unsupervised learning)

$$\begin{array}{c|c} r & d \\ \hline r \\ \cdot \\ n \end{array}$$
 'Low-rank'

## Big *n* and Big *d*

### We need methods that are linear in time and space

### One idea: Exploit sparsity

- computational gains

### Another idea: Use different algorithms

• Gradient descent is an iterative algorithm that requires O(nd) computation and O(d)local storage per iteration

• Explicit sparsity can provide orders of magnitude storage and

• Latent sparsity assumption can be used to reduce dimension, e.g., PCA, low-rank approximation (unsupervised learning)



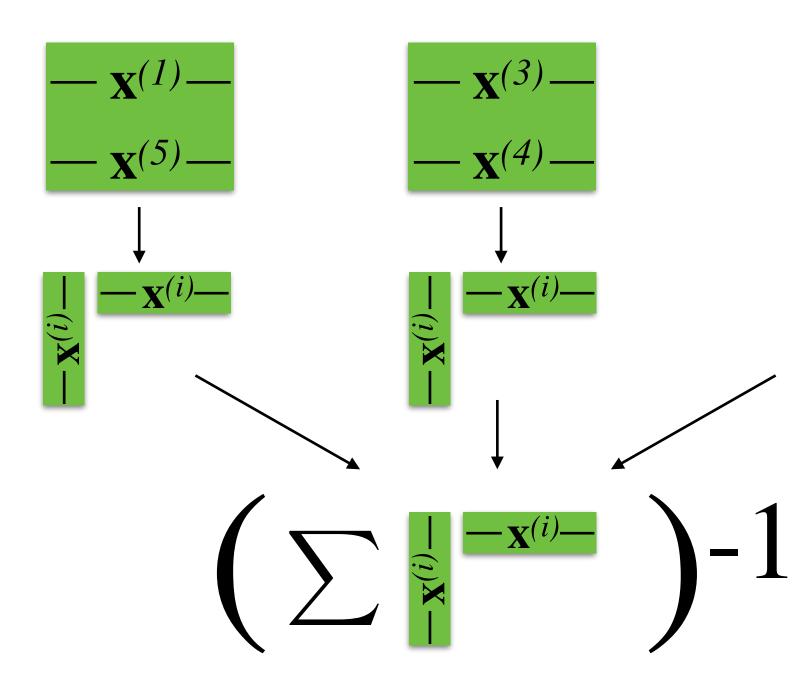
### Closed Form Solution for Big n and Big d

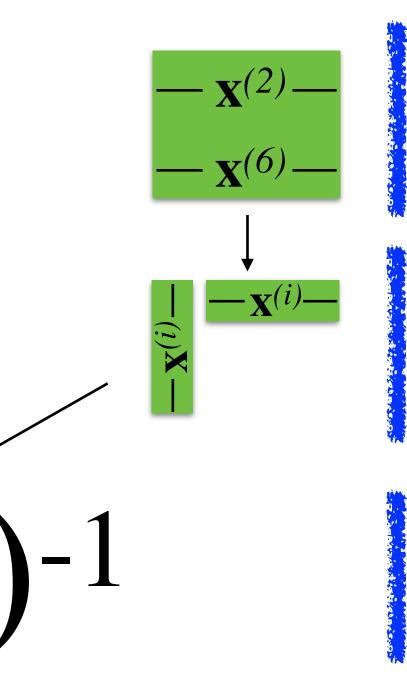
#### Example: n = 6; 3 workers

workers:

map:

reduce:





O(*nd*) Distributed Storage

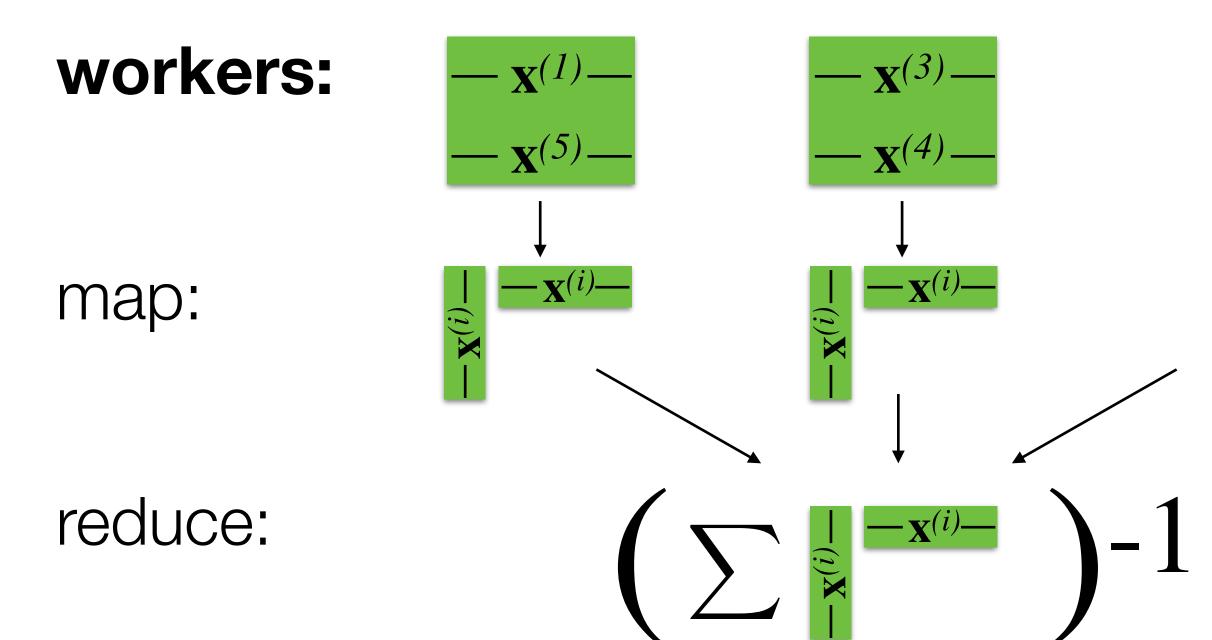
O(*nd*<sup>2</sup>) Distributed Computation

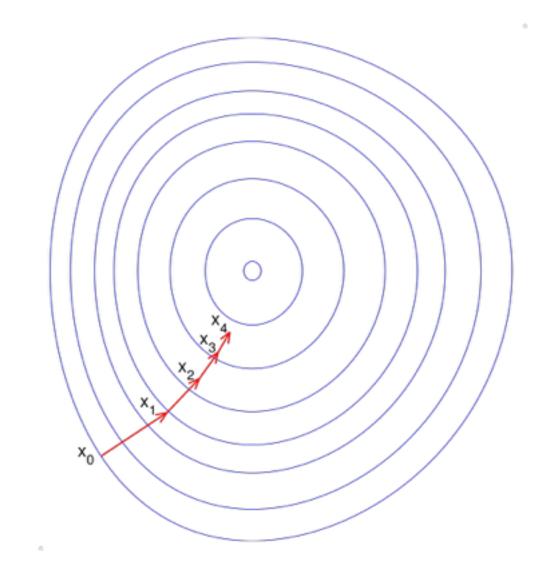
O(d<sup>2</sup>) Local Storage

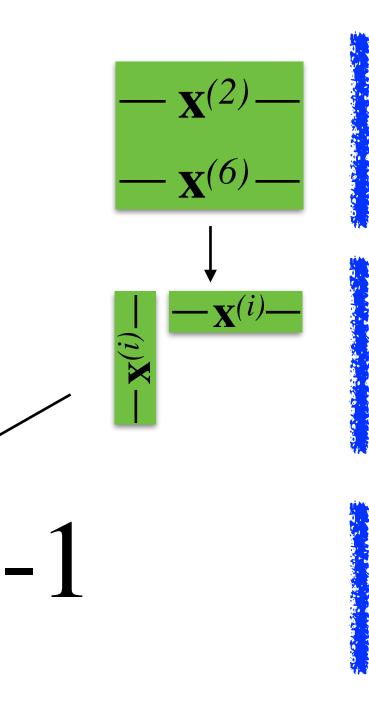
 $O(d^3)$  Local  $O(d^2)$  Local Computation Storage

# Gradient Descent for Big *n* and Big *d*

#### Example: n = 6; 3 workers







O(*nd*) Distributed Storage

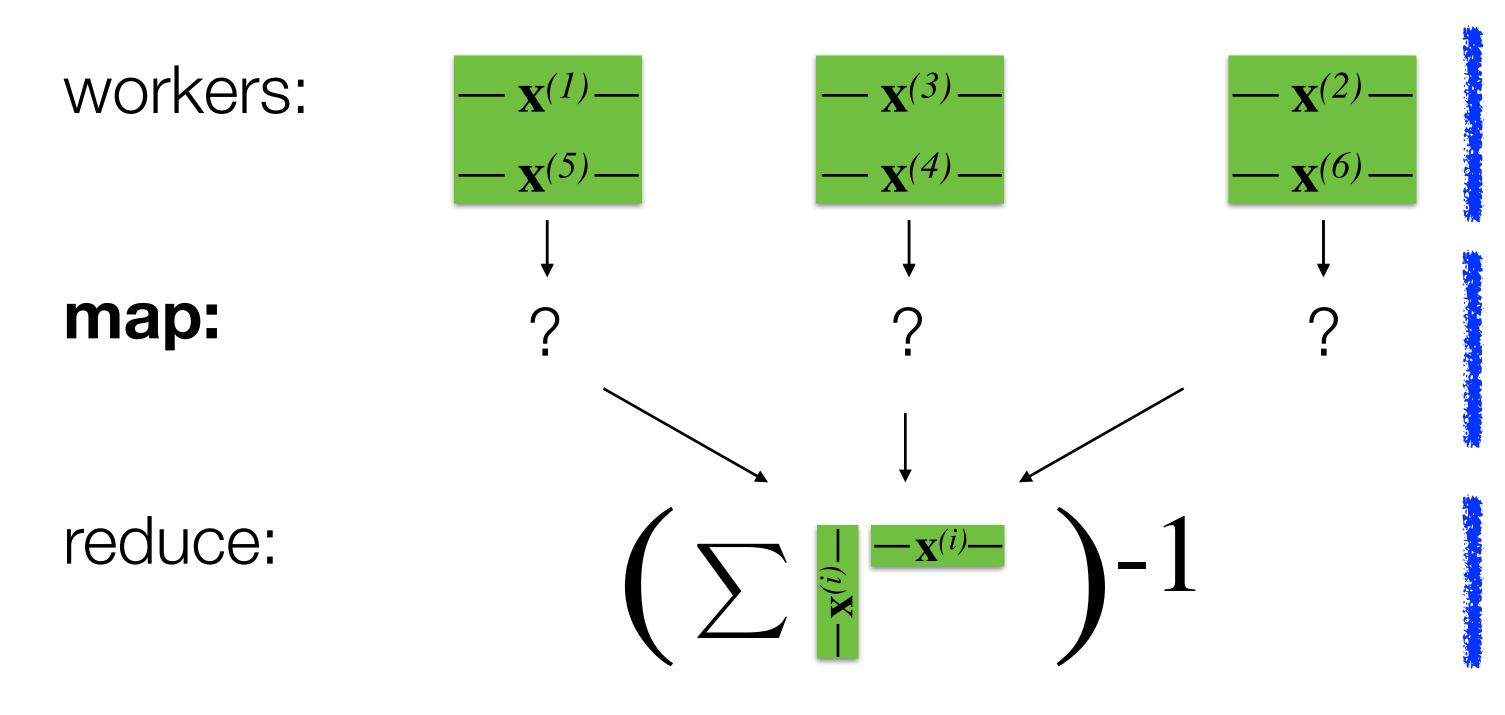
O(*nd*<sup>2</sup>) Distributed Computation

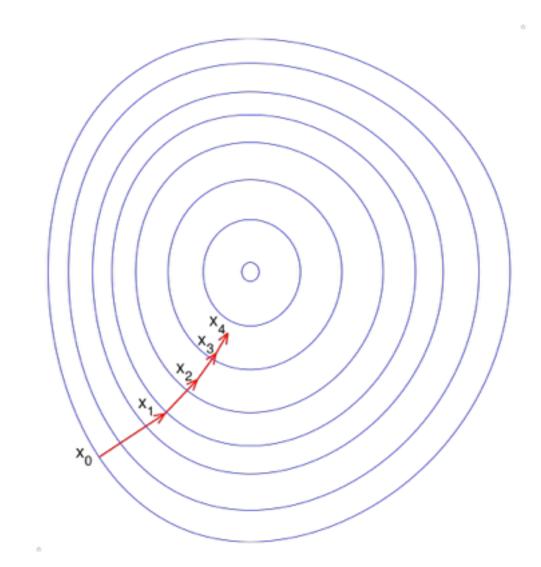
O(d<sup>2</sup>) Local Storage

 $O(d^3)$  Local  $O(d^2)$  Local Computation Storage

# Gradient Descent for Big *n* and Big *d*

#### Example: n = 6; 3 workers



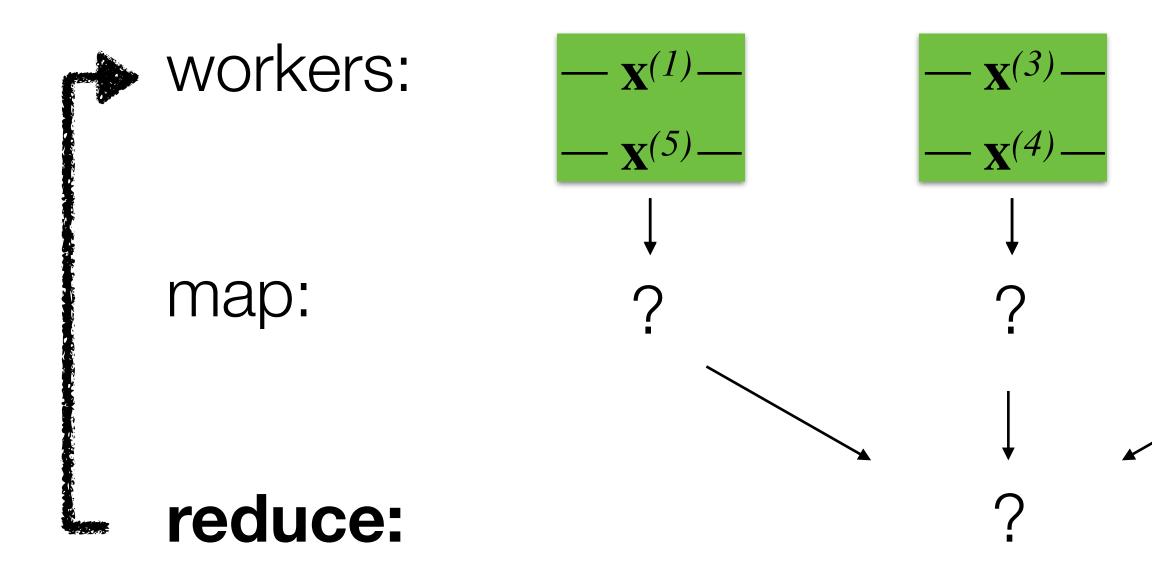


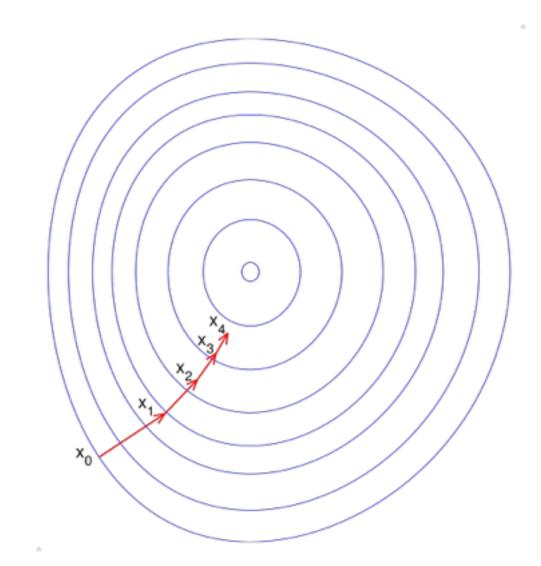
O(nd) Distributed Storage O(nd) $O(nd^2)$ Distributed Computation O(d) $O(d^2)$  Local Storage

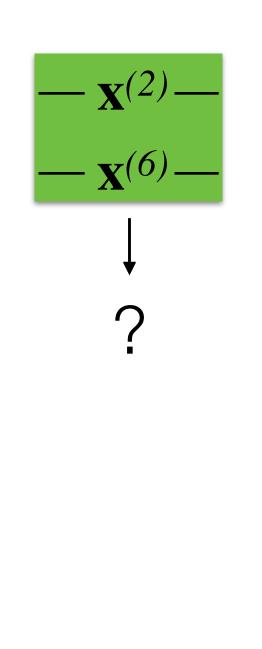
 $O(d^3)$  Local  $O(d^2)$  Local Computation Storage

# Gradient Descent for Big *n* and Big *d*

#### Example: n = 6; 3 workers







O(nd) Distributed Storage O(nd) $O(nd^2)$ Distributed Computation O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)Storage O(d)O(d)O(d)Storage O(d)O(d)O(d)Storage O(d)O(d)O(d)Storage O(d)O(d)Storage O(d)O(d)Storage O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O(d)O