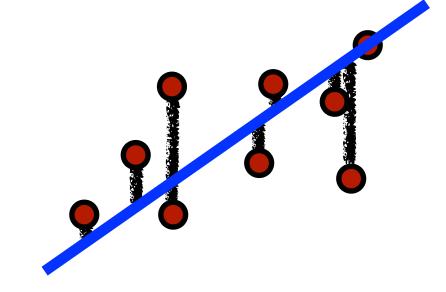
Linear Regression





Regression

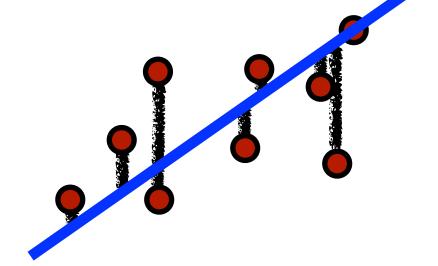


Goal: Learn a mapping from observations (features) to continuous labels given a training set (supervised learning)

Example: Height, Gender, Weight → Shoe Size

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

Linear Least Squares Regression



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

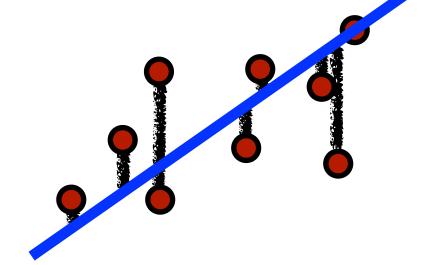
For each observation we have a feature vector, x, and label, y

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

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

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

Linear Least Squares Regression



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

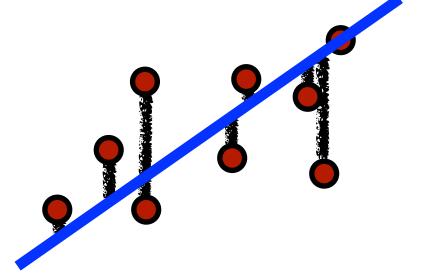
We can augment the feature vector to incorporate offset:

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

We can then rewrite this linear mapping as scalar product:

$$y \approx \hat{y} = \sum_{i=0}^{3} w_i x_i = \mathbf{w}^{\mathsf{T}} \mathbf{x}$$

Why a Linear Mapping?



Simple

Often works well in practice

Can introduce complexity via feature extraction

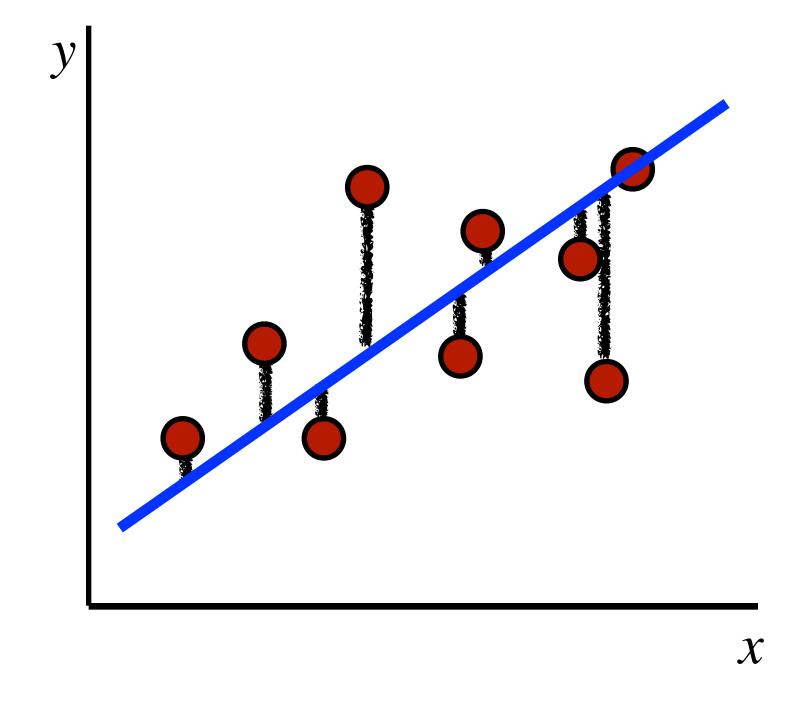
1D Example

Goal: find the line of best fit

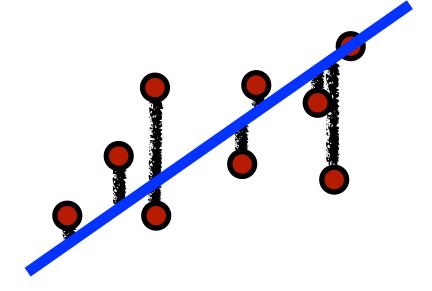
x coordinate: features

y coordinate: labels

$$y \approx \hat{y} = w_0 + w_1 x$$
Intercept / Offset Slope



Evaluating Predictions



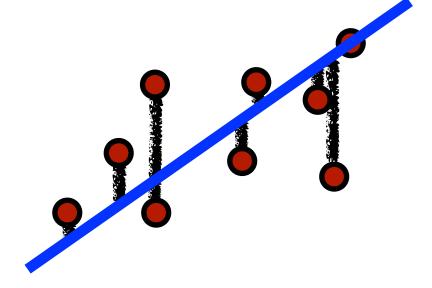
Can measure 'closeness' between label and prediction

- 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: $(y \hat{y})^2$ \leftarrow Has nice mathematical properties

How Can We Learn Model (w)?



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

Recall two earlier points:

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

Idea: Find w that minimizes squared loss over training points:

$$\min_{\mathbf{w}} \sum_{i=1}^{n} (\underline{\mathbf{w}}^{\top} \mathbf{x}^{(i)} - y^{(i)})^{2}$$

Given n training points with d features, we define:

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

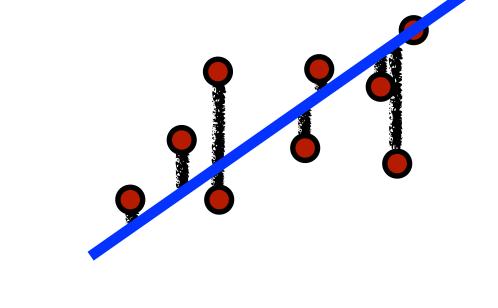
Least Squares Regression: Learn mapping (w) from features to labels that minimizes residual sum of squares:

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

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

Find solution by setting derivative to zero

1D:
$$f(w) = ||w\mathbf{x} - \mathbf{y}||_2^2 = \sum_{i=1}^n (wx^{(i)} - y^{(i)})^2$$



$$\frac{df}{dw}(w) = 2\sum_{i=1}^{n} x^{(i)}(wx^{(i)} - y^{(i)}) = 0 \iff w\mathbf{x}^{\top}\mathbf{x} - \mathbf{x}^{\top}\mathbf{y} = 0$$
$$\iff w = (\mathbf{x}^{\top}\mathbf{x})^{-1}\mathbf{x}^{\top}\mathbf{y}$$

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

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

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

Overfitting and Generalization

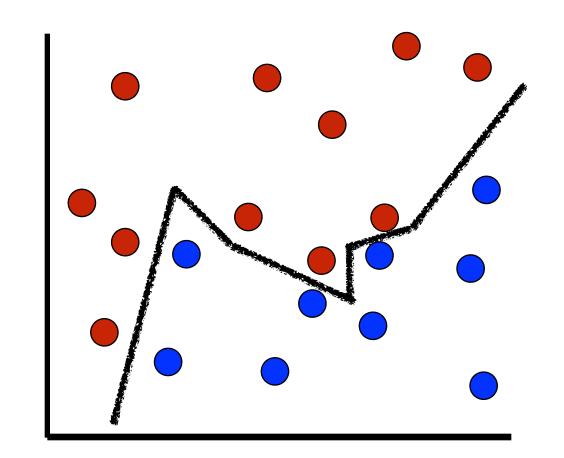
We want good predictions on new data, i.e., 'generalization'

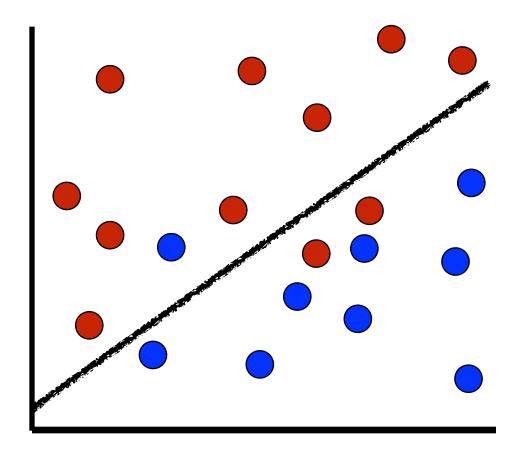
Least squares regression minimizes training error, and could overfit

• 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





Given n training points with d features, we define:

- $\mathbf{X} \in \mathbb{R}^{n \times d}$: matrix storing points
- $\mathbf{y} \in \mathbb{R}^n$: real-valued labels
- $oldsymbol{\hat{y}} \in \mathbb{R}^n$: predicted labels, where $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$
- ullet $\mathbf{w} \in \mathbb{R}^d$: regression parameters / model to learn

Ridge Regression: Learn mapping (w) that minimizes residual sum of squares along with a regularization term:

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

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

free parameter trades off between training error and model complexity

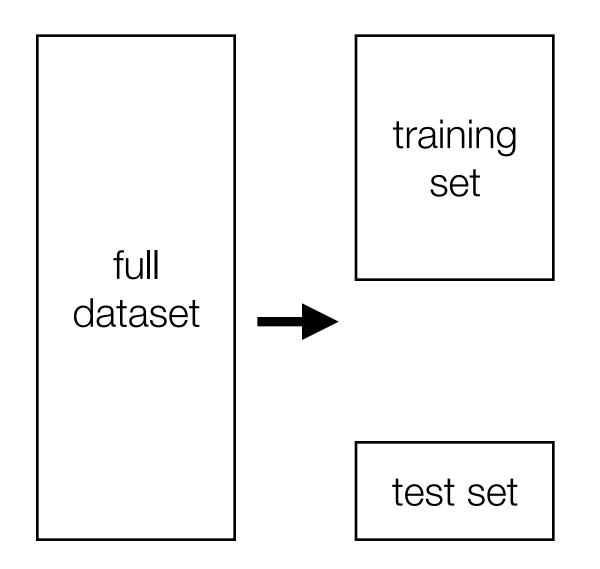
Millionsong Regression Pipeline





full dataset

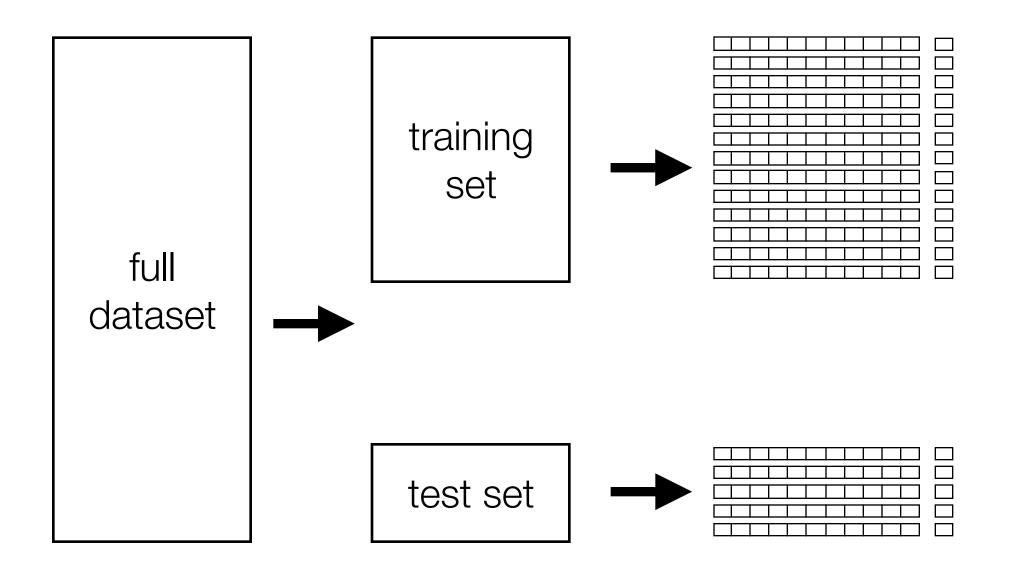
Obtain Raw Data

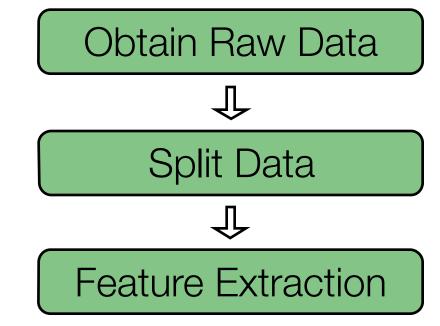


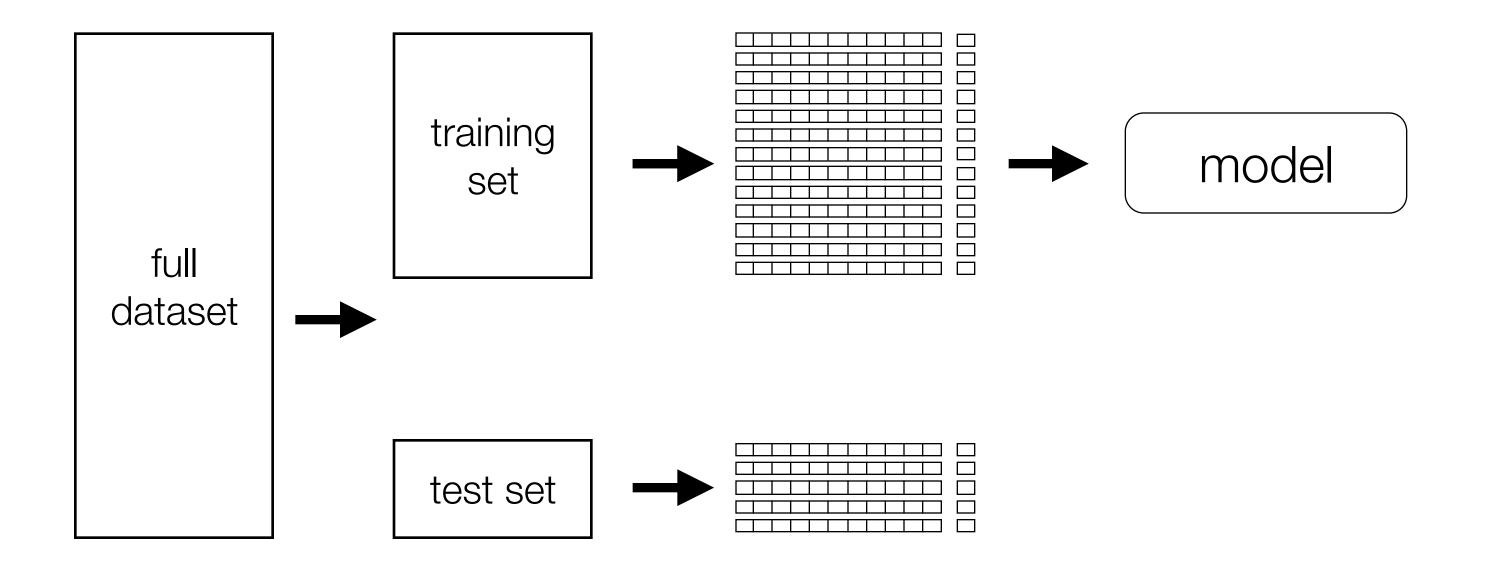
Obtain Raw Data

U

Split Data











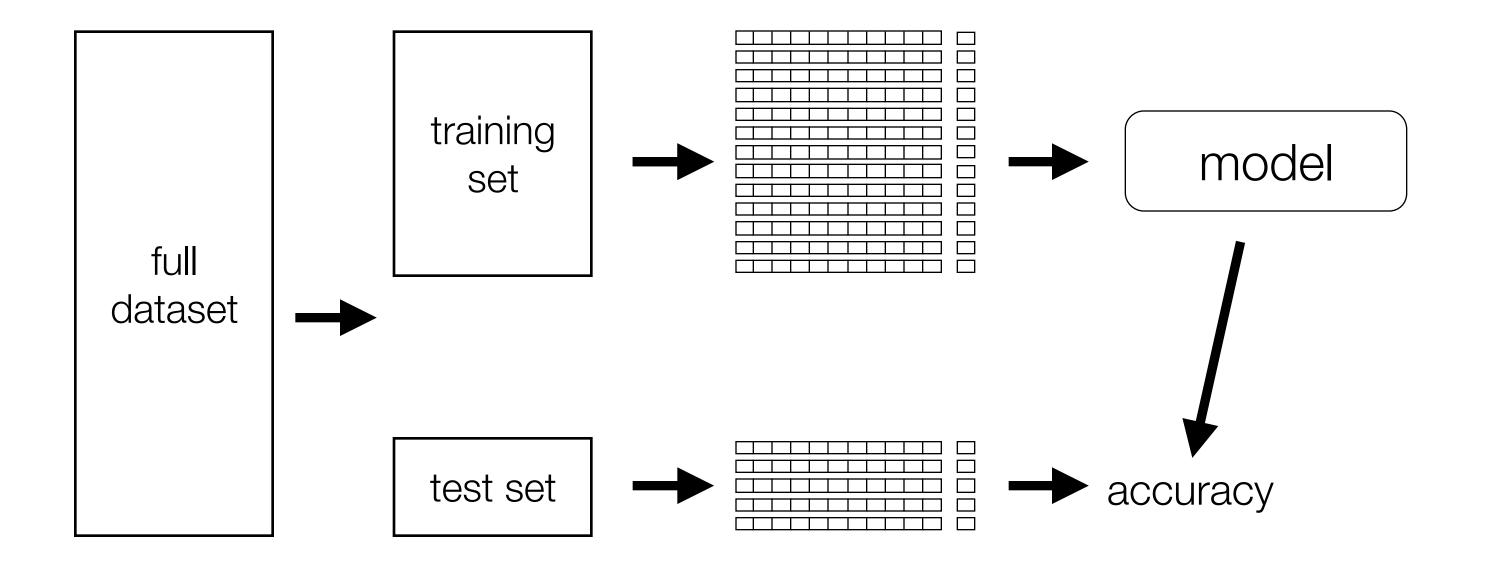
Split Data



Feature Extraction



Supervised Learning







Split Data



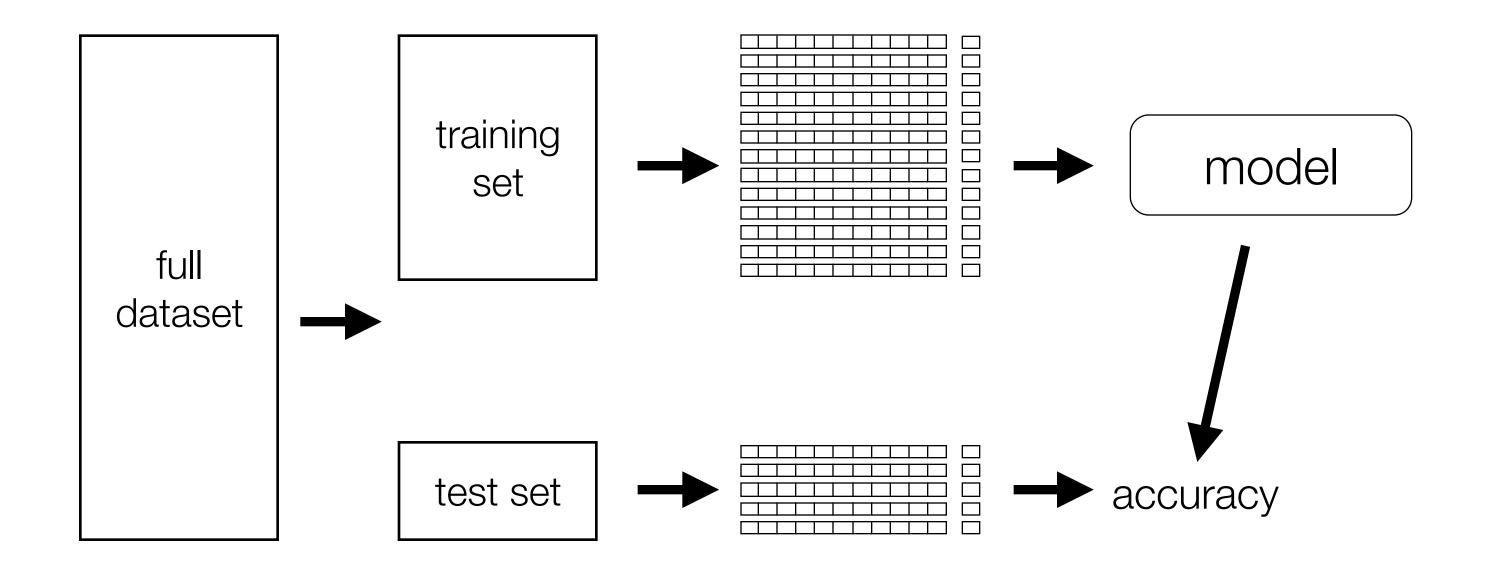
Feature Extraction

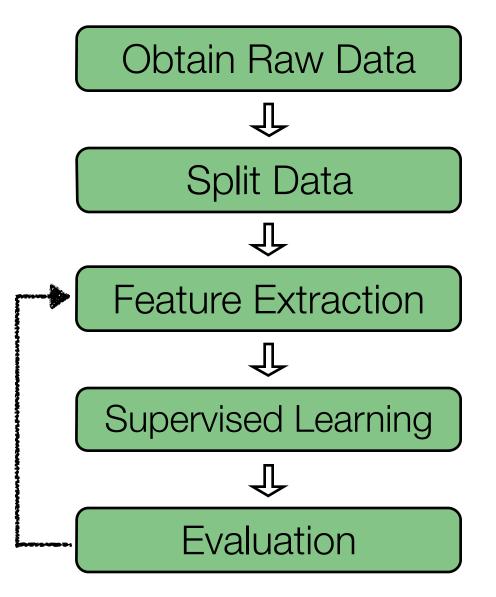


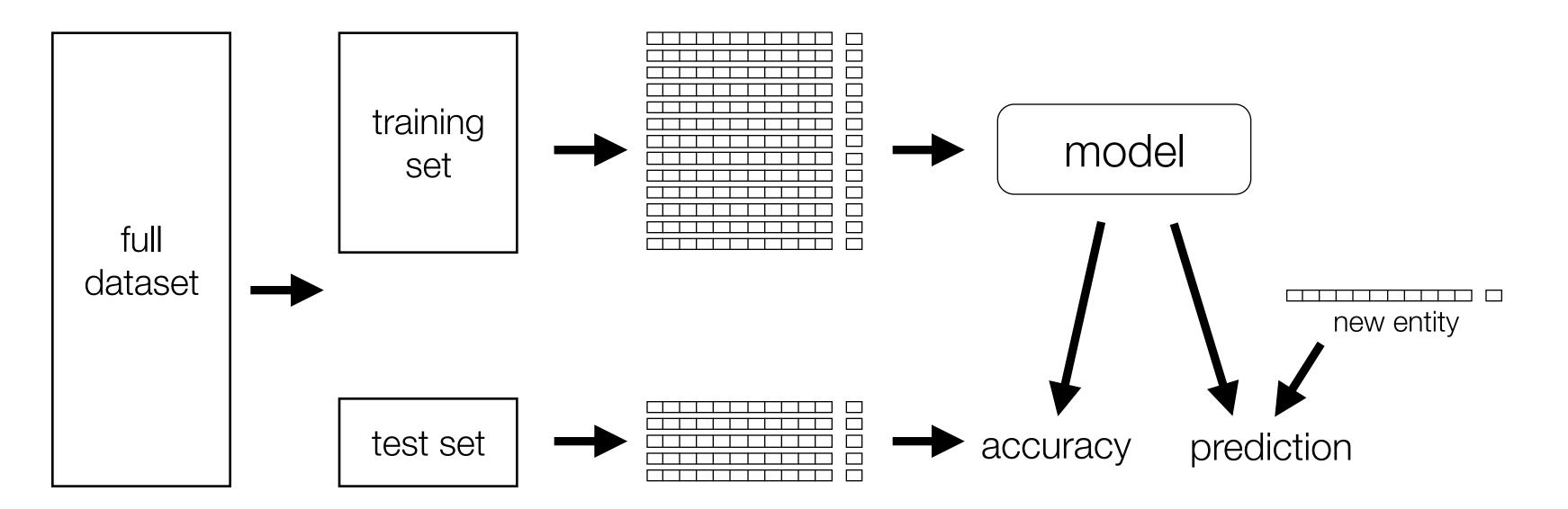
Supervised Learning

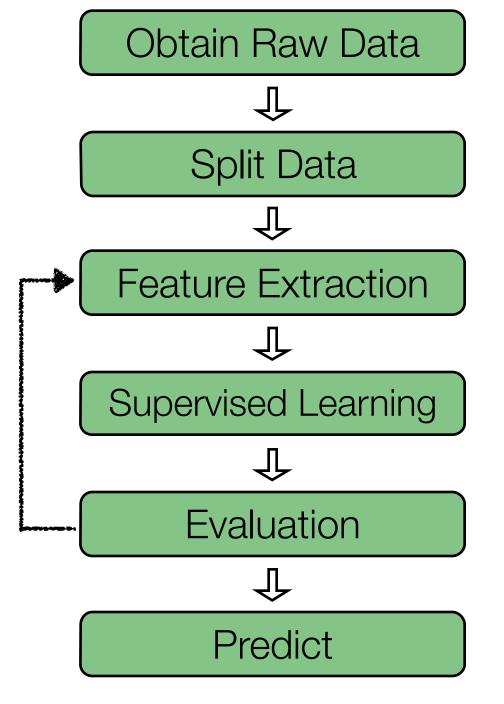


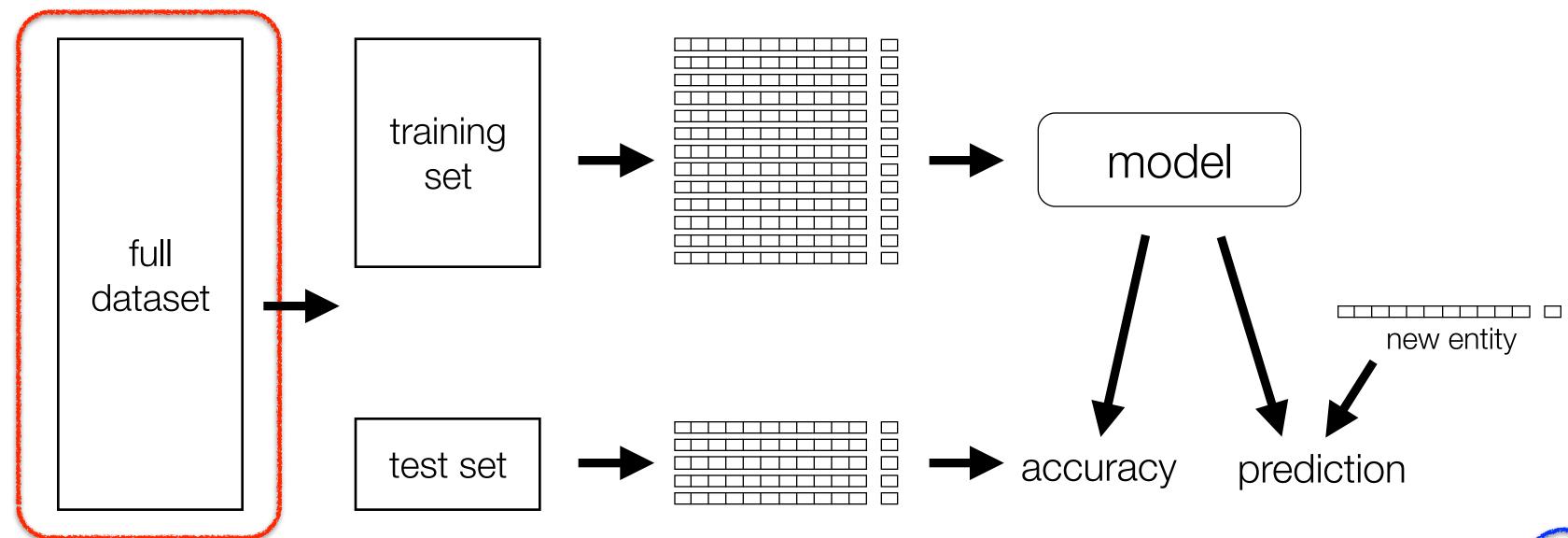
Evaluation







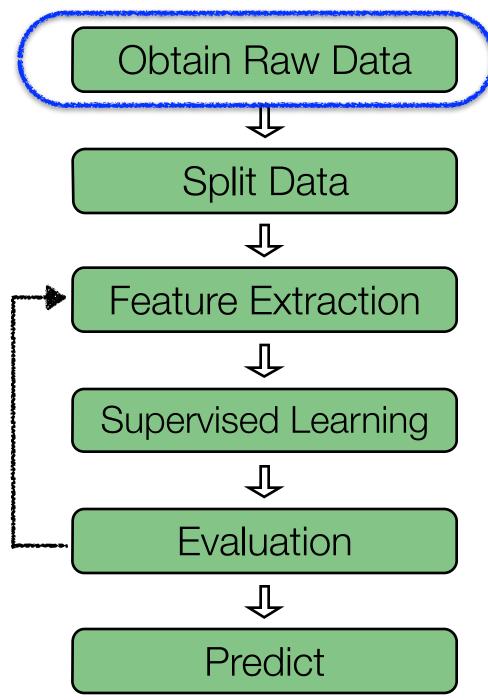


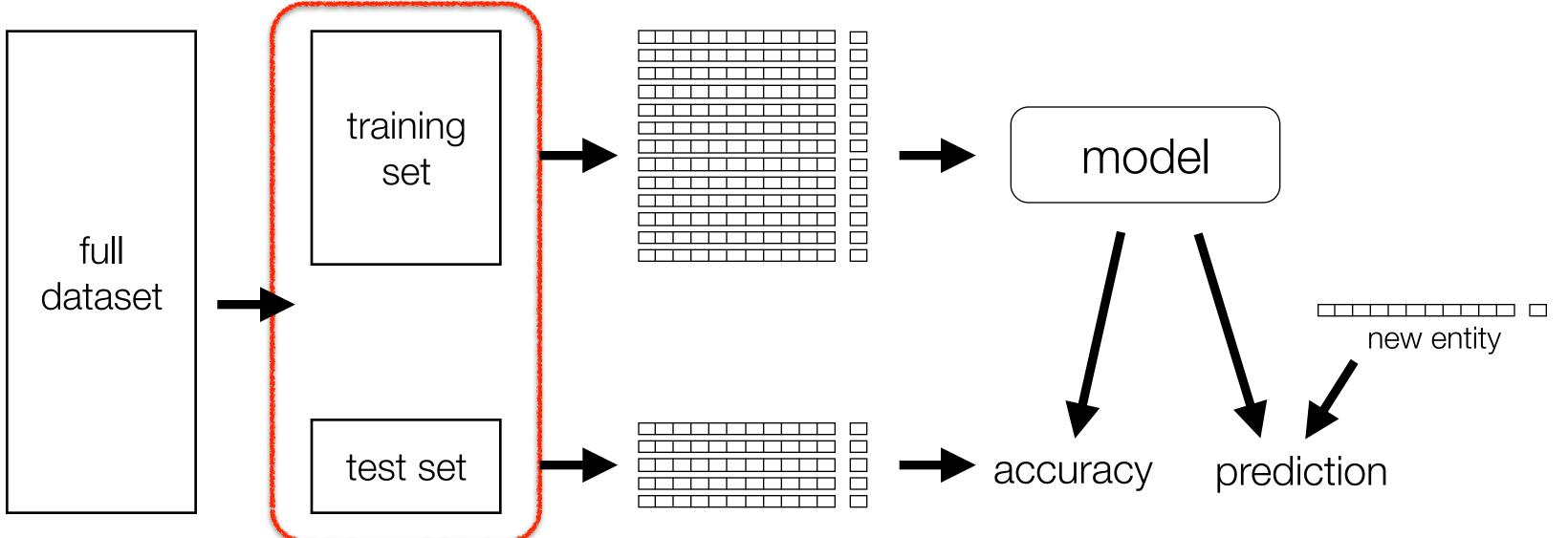


Goal: Predict song's release year from audio features

Raw Data: Millionsong Dataset from UCI ML Repository

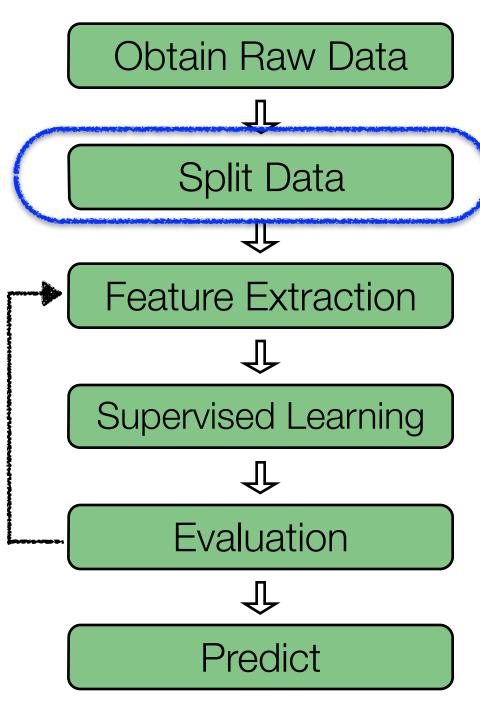
- Western, commercial tracks from 1980-2014
- 12 timbre averages (features) and release year (label)

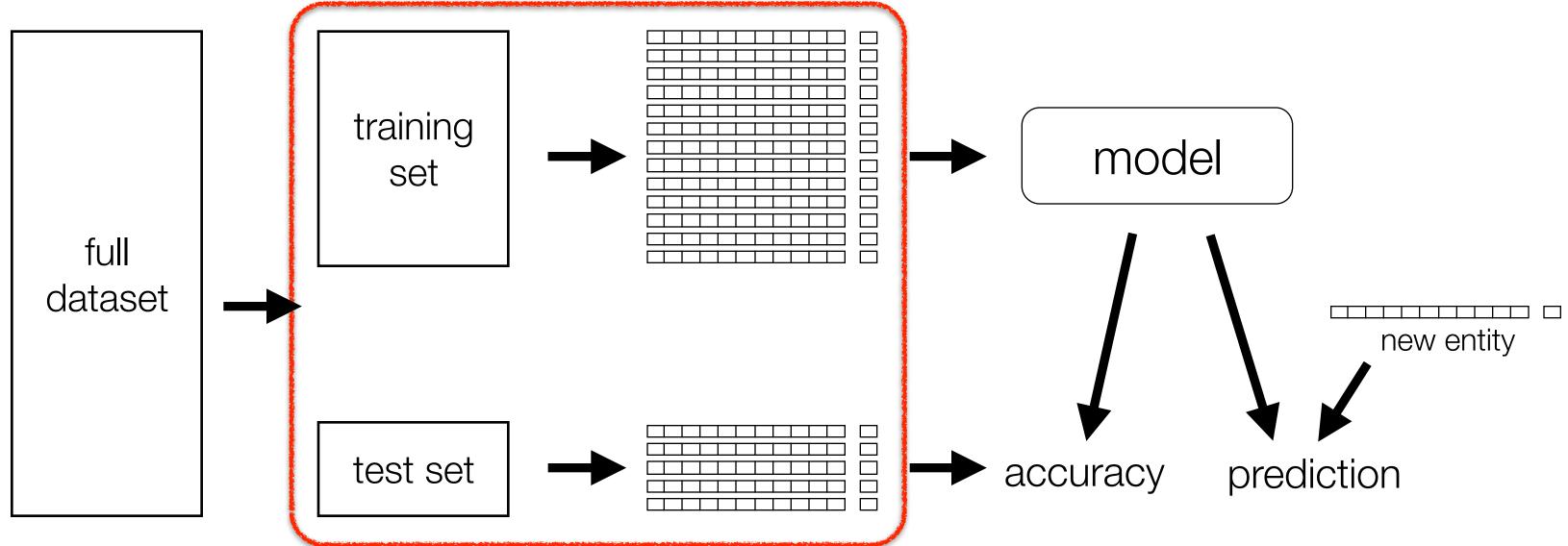




Split Data: Train on training set, evaluate with test set

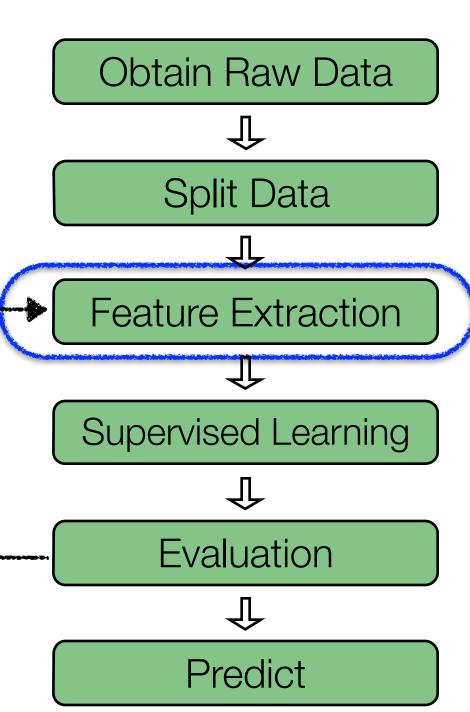
- Test set simulates unobserved data
- Test error tells us whether we've generalized well





Feature Extraction: Quadratic features

- Compute pairwise feature interactions
- Captures covariance of initial timbre features
- Leads to a non-linear model relative to raw features



Given 2 dimensional data, quadratic features are:

$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top \implies \Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 & x_1 x_2 & x_2 x_1 & x_2^2 \end{bmatrix}^\top$$

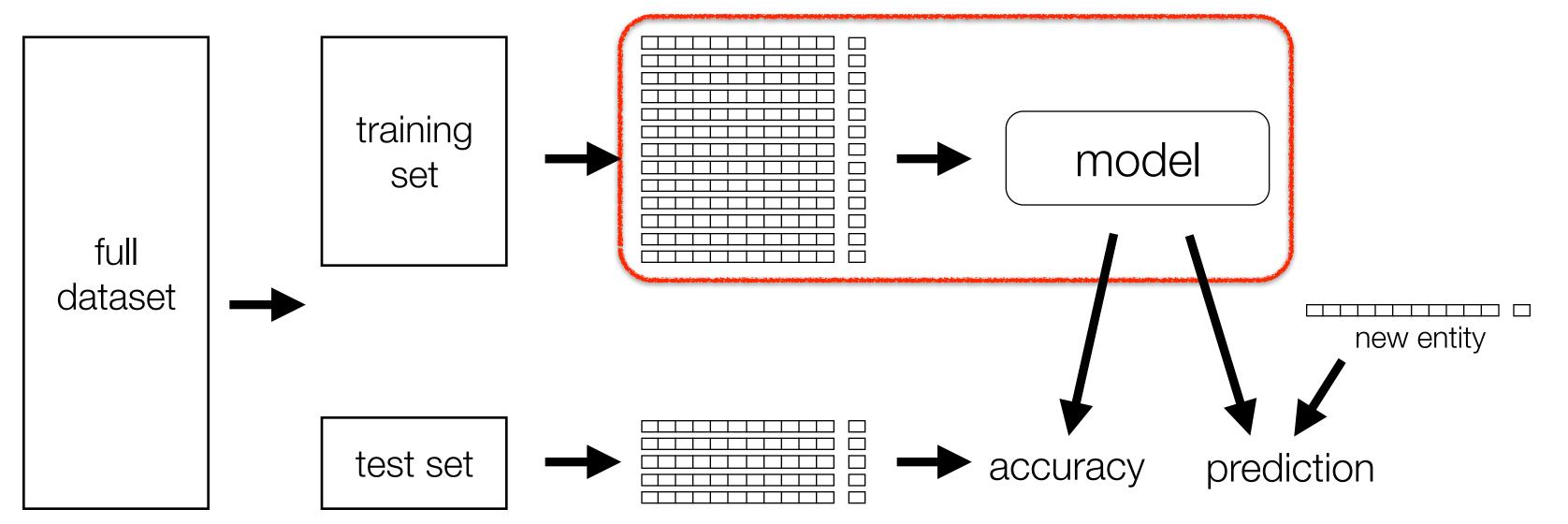
$$\mathbf{z} = \begin{bmatrix} z_1 & z_2 \end{bmatrix}^\top \implies \Phi(\mathbf{z}) = \begin{bmatrix} z_1^2 & z_1 z_2 & z_2 z_1 & z_2^2 \end{bmatrix}^\top$$

More succinctly:

$$\Phi'(\mathbf{x}) = \begin{bmatrix} x_1^2 & \sqrt{2}x_1x_2 & x_2^2 \end{bmatrix}^{\top} \qquad \Phi'(\mathbf{z}) = \begin{bmatrix} z_1^2 & \sqrt{2}z_1z_2 & z_2^2 \end{bmatrix}^{\top}$$

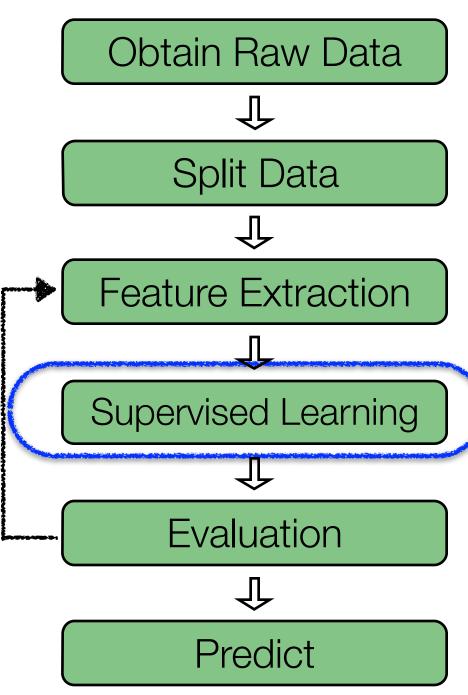
Equivalent inner products:

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



Supervised Learning: Least Squares Regression

- Learn a mapping from entities to continuous labels given a training set
- Audio features → Song year



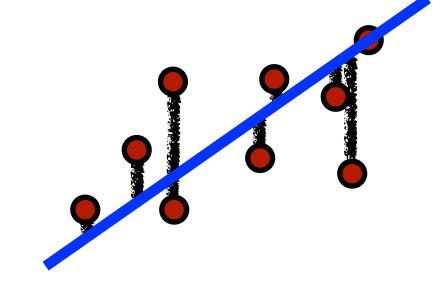
Given n training points with d features, we define:

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

Ridge Regression: Learn mapping (w) that minimizes residual sum of squares along with a regularization term:

$$\min_{\mathbf{w}} \frac{\text{Training Error}}{||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2} + \frac{\text{Model Complexity}}{\lambda ||\mathbf{w}||_2^2}$$

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



Ridge Regression: Learn mapping (w) that minimizes residual sum of squares along with a regularization term:

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

free parameter trades off between training . error and model complexity

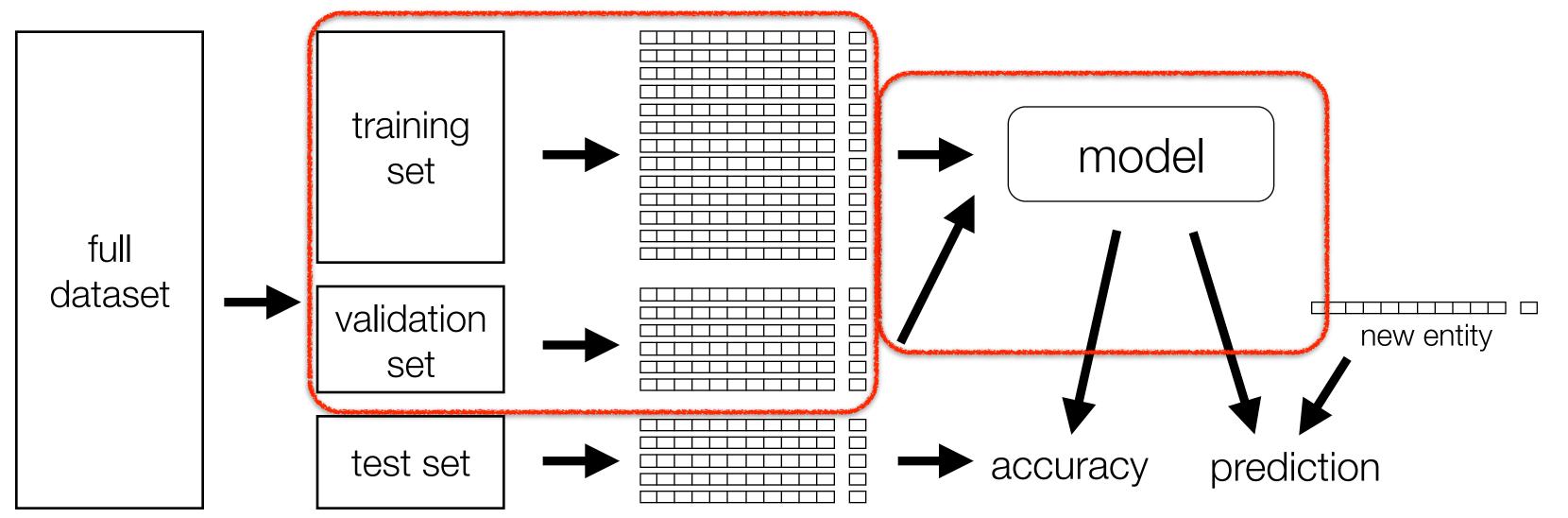
How do we choose a good value for this free parameter?

Most methods have free parameters / 'hyperparameters' to tune

First thought: Search over multiple values, evaluate each on test set

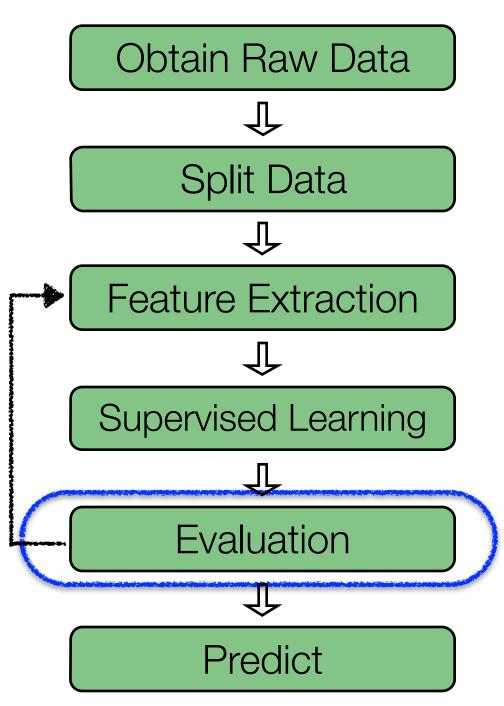
- But, goal of test set is to simulate unobserved data
- We may overfit if we use it to choose hyperparameters

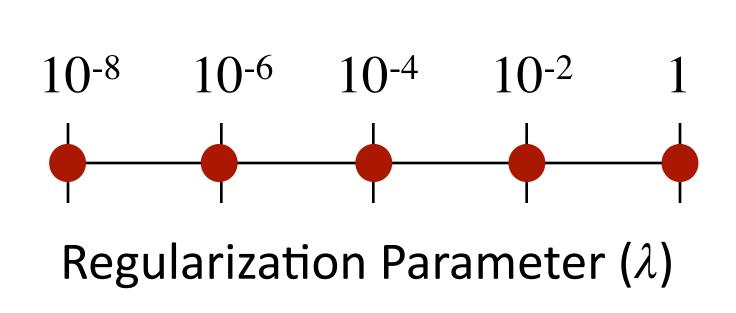
Second thought: Create another hold out dataset for this search

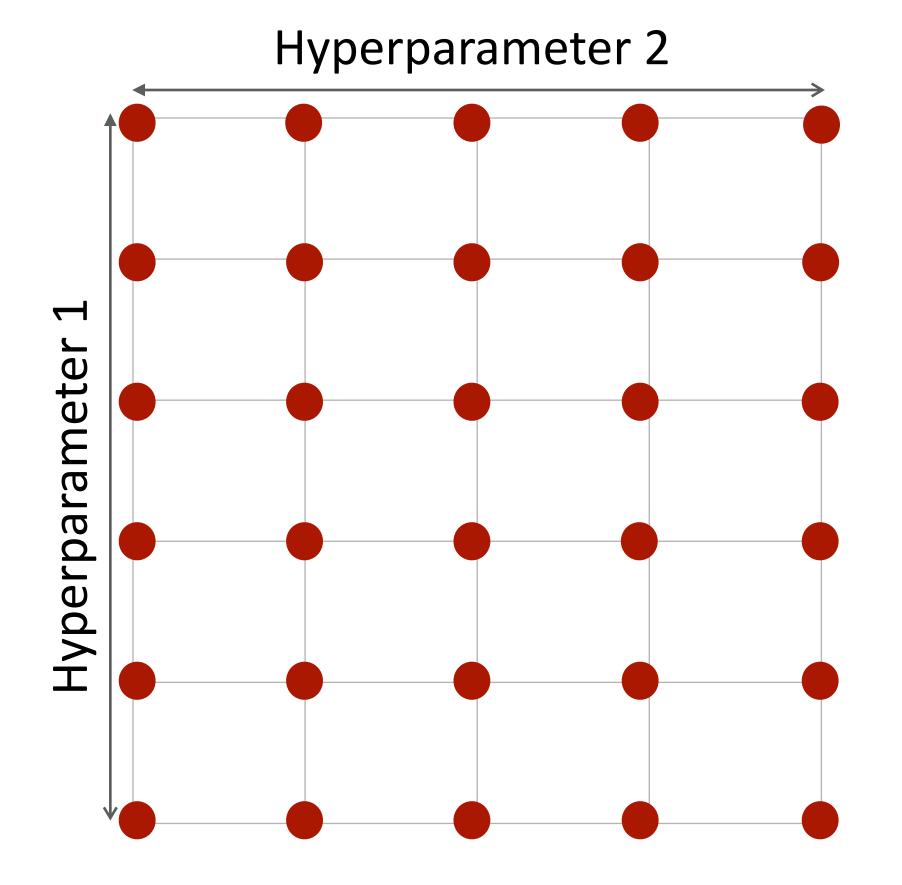


Evaluation (Part 1): Hyperparameter tuning

- Training: train various models
- Validation: evaluate various models (e.g., Grid Search)
- Test: evaluate final model's accuracy



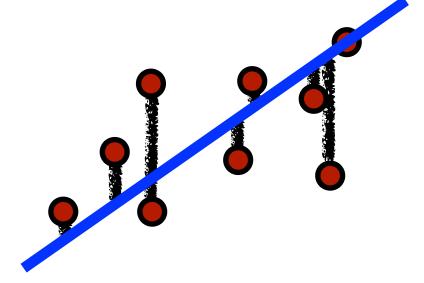




Grid Search: Exhaustively search through hyperparameter space

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

Evaluating Predictions



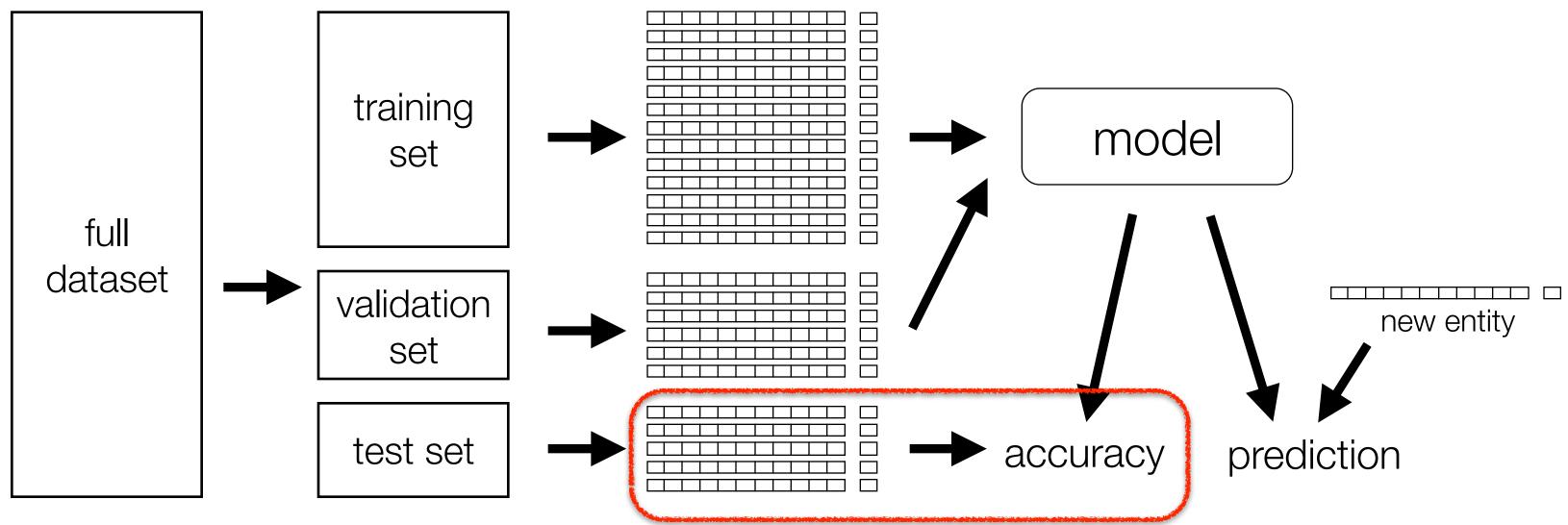
How can we compare labels and predictions for n validation points?

Least squares optimization involves squared loss, $(y - \hat{y})^2$, so it seems reasonable to use mean squared error (**MSE**):

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

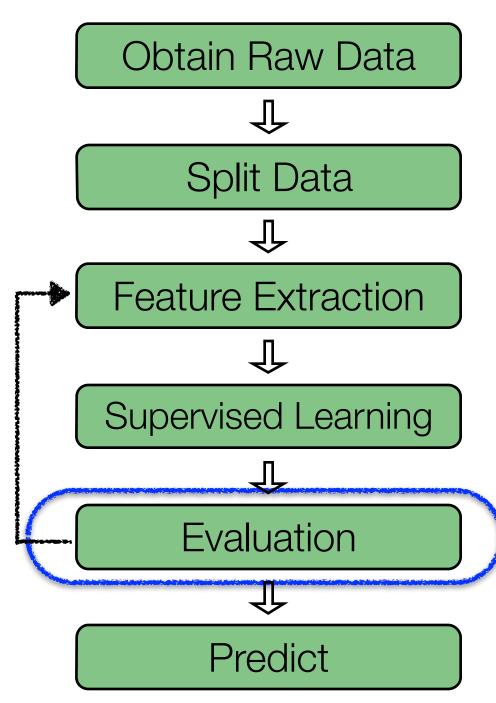
But MSE's unit of measurement is square of quantity being measured, e.g., "squared years" for song prediction

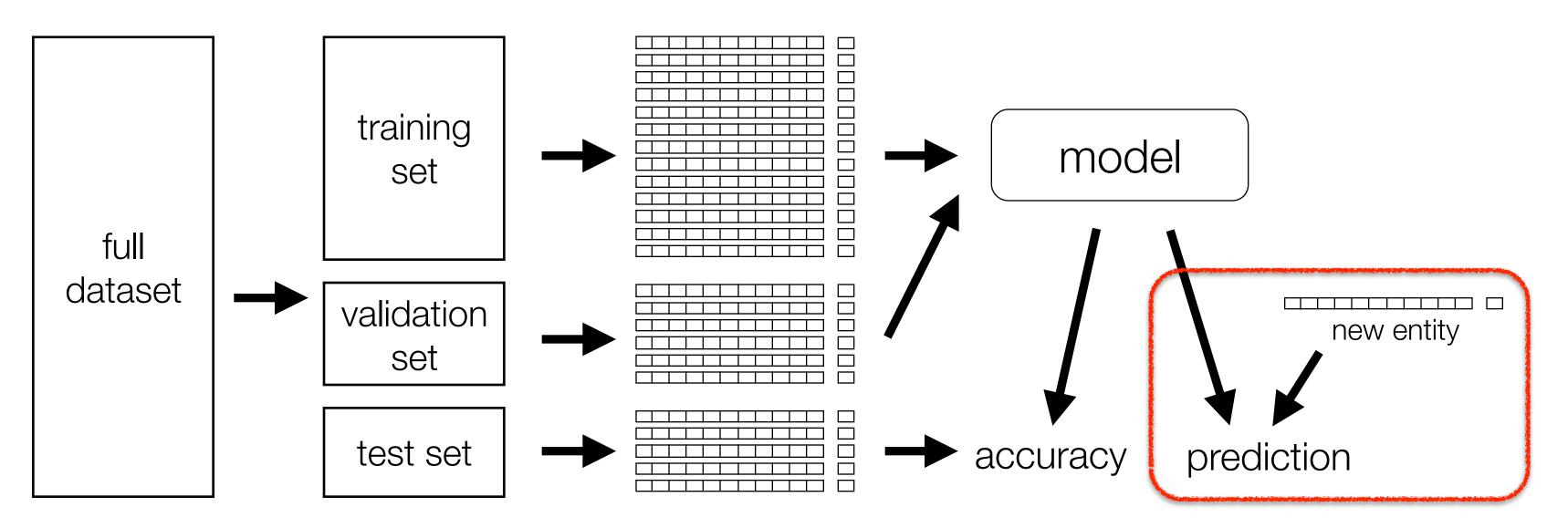
More natural to use root-mean-square error (**RMSE**), i.e., \sqrt{MSE}



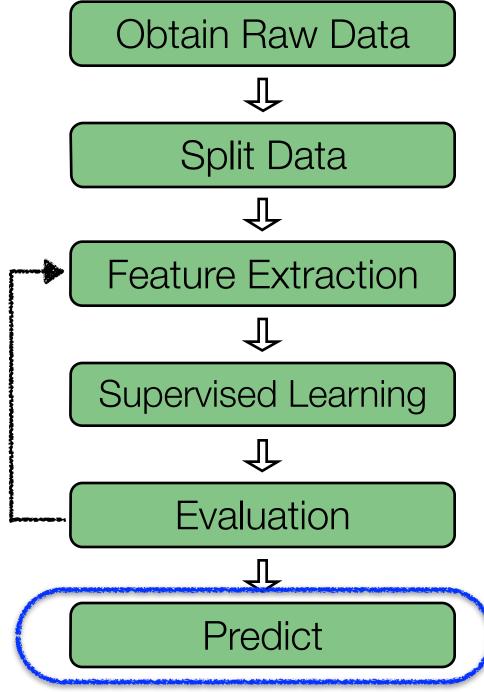
Evaluation (Part 2): Evaluate final model

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





Predict: Final model can then be used to make predictions on future observations, e.g., new songs



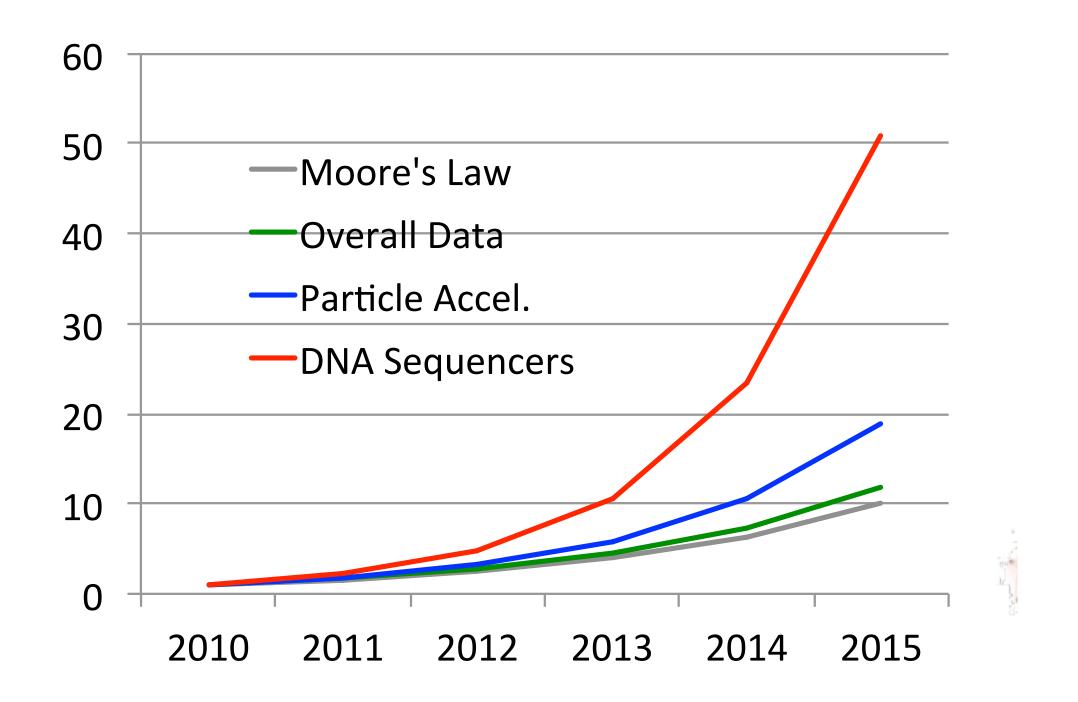
Distributed ML: Computation and Storage



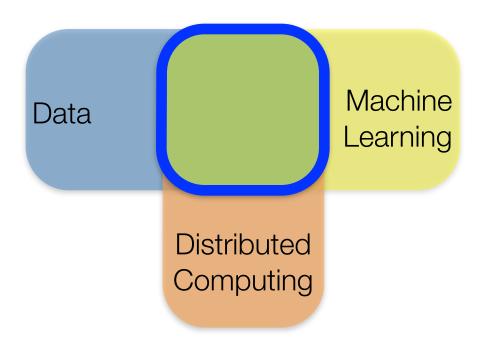


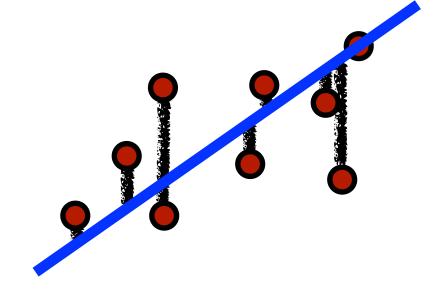
Challenge: Scalability

Classic ML techniques are not always suitable for modern datasets



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





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

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

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

How do we solve this computationally?

Computational profile similar for Ridge Regression

Computing Closed Form Solution

$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

Computational bottlenecks:

- Matrix multiply of $\mathbf{X}^{\top}\mathbf{X}$: $O(nd^2)$ operations
- Matrix inverse: $O(d^3)$ operations

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

Storage Requirements

$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

Consider storing values as floats (8 bytes)

Storage bottlenecks:

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

Big n and Small d

$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

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

Storing X and computing $X^{T}X$ are the bottlenecks

Can distribute storage and computation!

- Store data points (rows of X) across machines
- ullet Compute $\mathbf{X}^{\mathsf{T}}\mathbf{X}$ as a sum of outer products

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

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 \\ \end{bmatrix}$$

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

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

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 & 18 \\ \end{bmatrix}$$

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

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 & 18 \\ 11 & 9 \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} \\ \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & -5 \end{bmatrix}$$

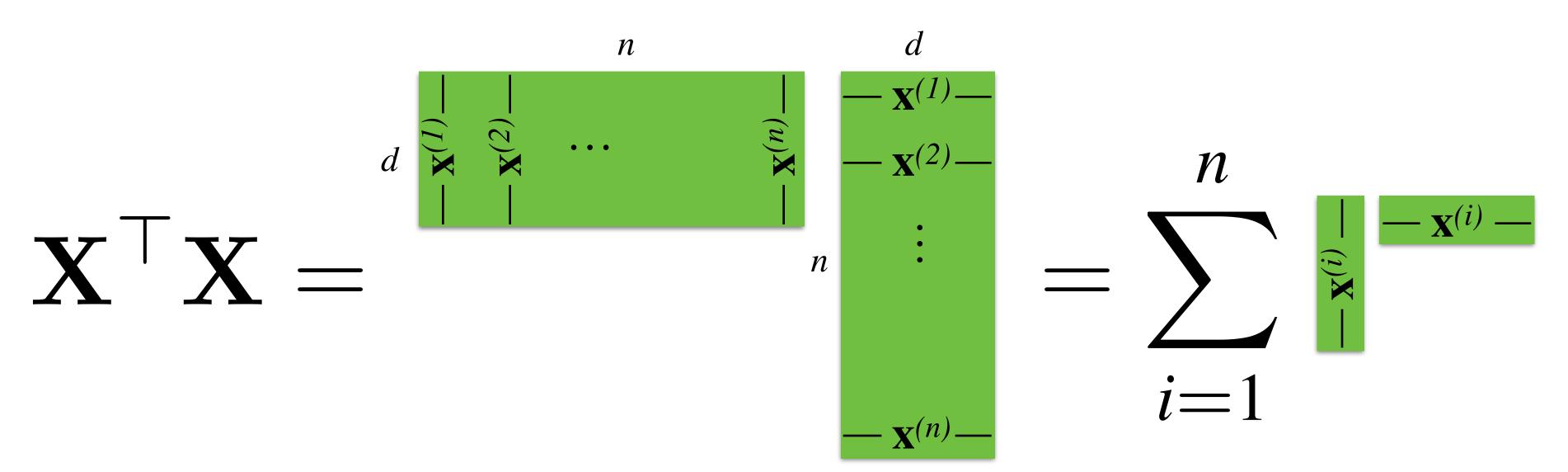
$$\begin{bmatrix} 9 & 18 \\ 4 & 8 \end{bmatrix} + \begin{bmatrix} 9 & -15 \\ 3 & -5 \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & 3 \end{bmatrix}$$

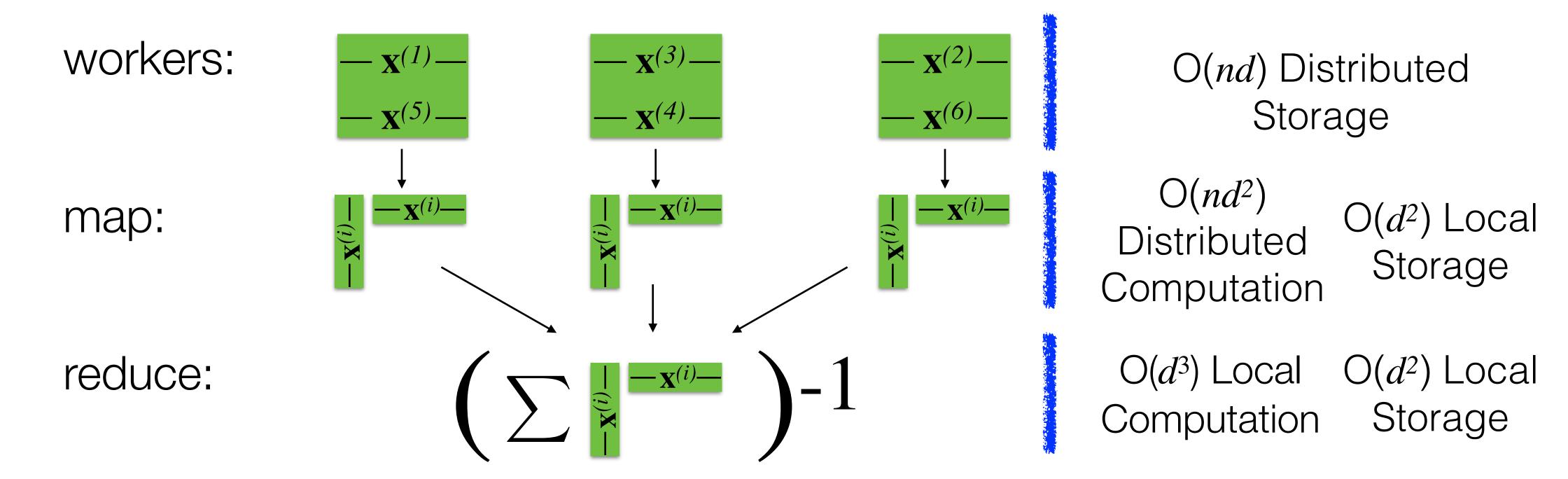
$$\begin{bmatrix} 9 & 18 \\ 4 & 8 \end{bmatrix} + \begin{bmatrix} 9 & -15 \\ 3 & -5 \end{bmatrix} + \begin{bmatrix} 10 & 15 \\ 4 & 6 \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 28 & 18 \\ 11 & 9 \end{bmatrix}$$

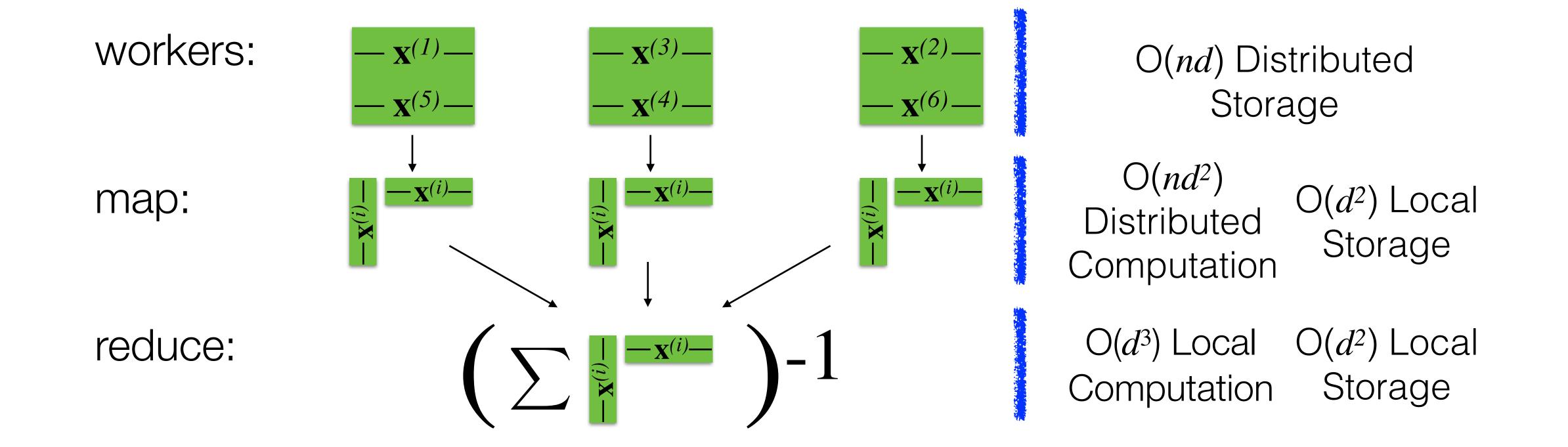
$$\begin{bmatrix} 9 & 18 \\ 4 & 8 \end{bmatrix} + \begin{bmatrix} 9 & -15 \\ 3 & -5 \end{bmatrix} + \begin{bmatrix} 10 & 15 \\ 4 & 6 \end{bmatrix}$$



Example: n = 6; 3 workers



trainData.map(computeOuterProduct) .reduce(sumAndInvert)



Distributed ML: Computation and Storage, Part II





Big n and Small d

$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

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

Can distribute storage and computation!

- Store data points (rows of X) across machines
- ullet Compute $\mathbf{X}^{\top}\mathbf{X}$ as a sum of outer products

Big n and Small d

$$\mathbf{w} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

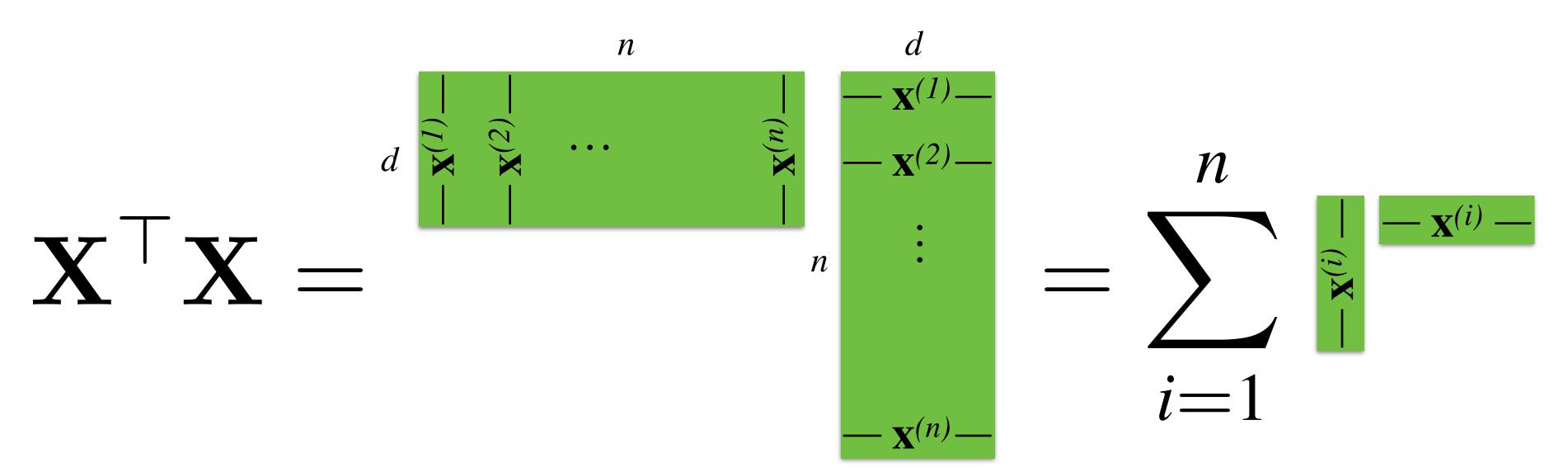
$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

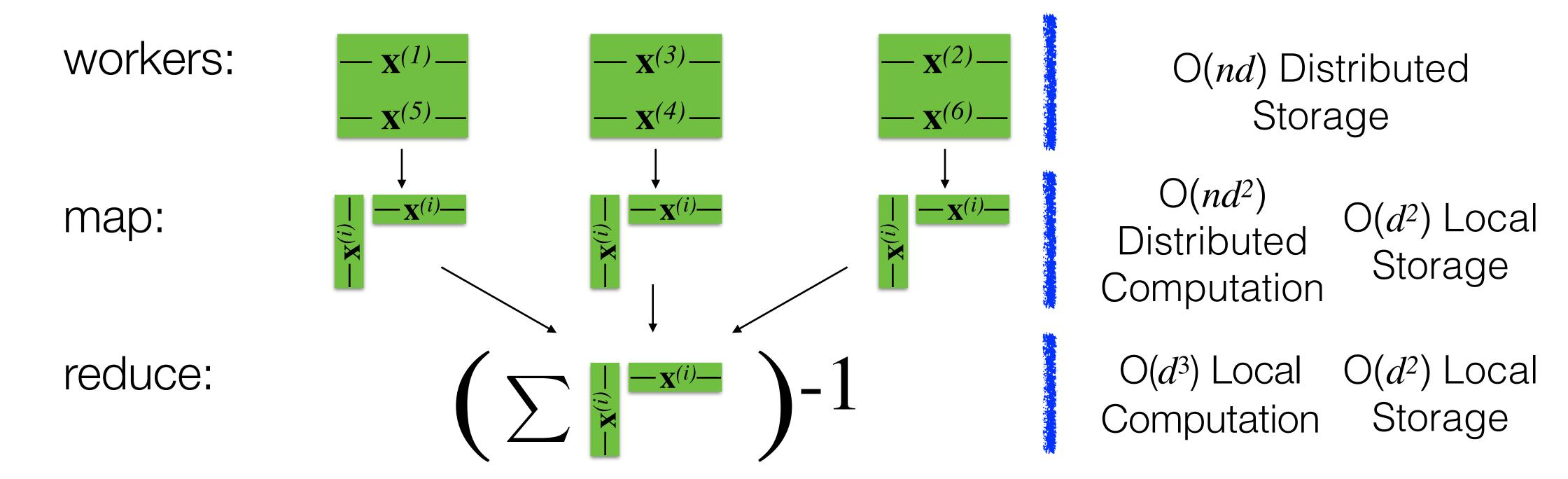
Storage: $O(nd + d^2)$ floats

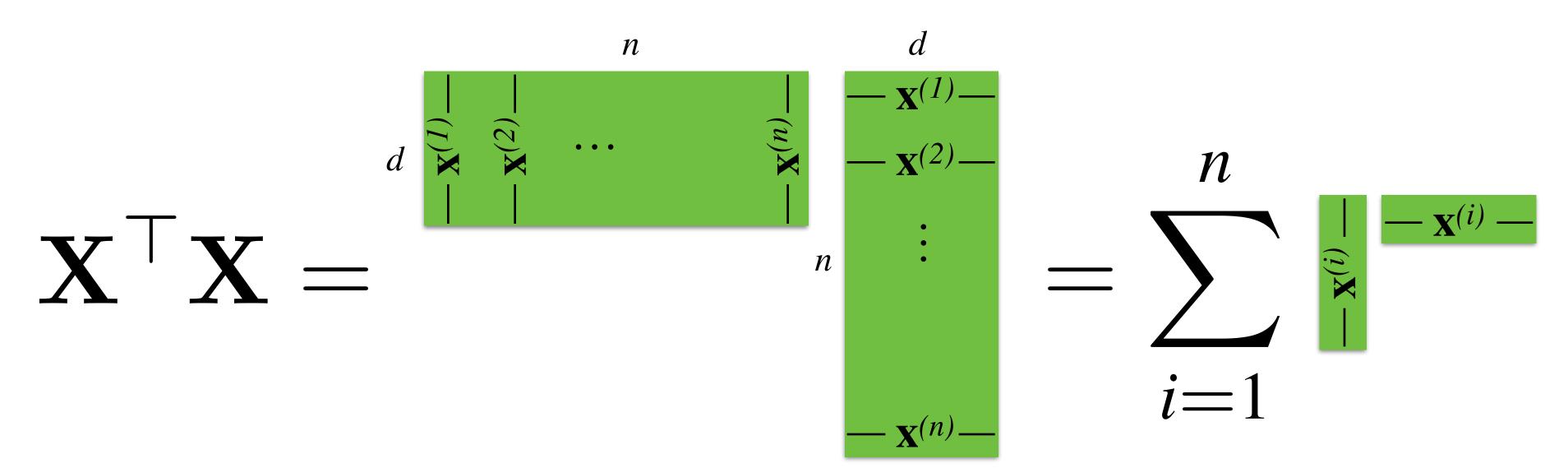
As before, storing \mathbf{X} and computing $\mathbf{X}^{\top}\mathbf{X}$ are bottlenecks Now, storing and operating on $\mathbf{X}^{\top}\mathbf{X}$ is also a bottleneck

Can't easily distribute!

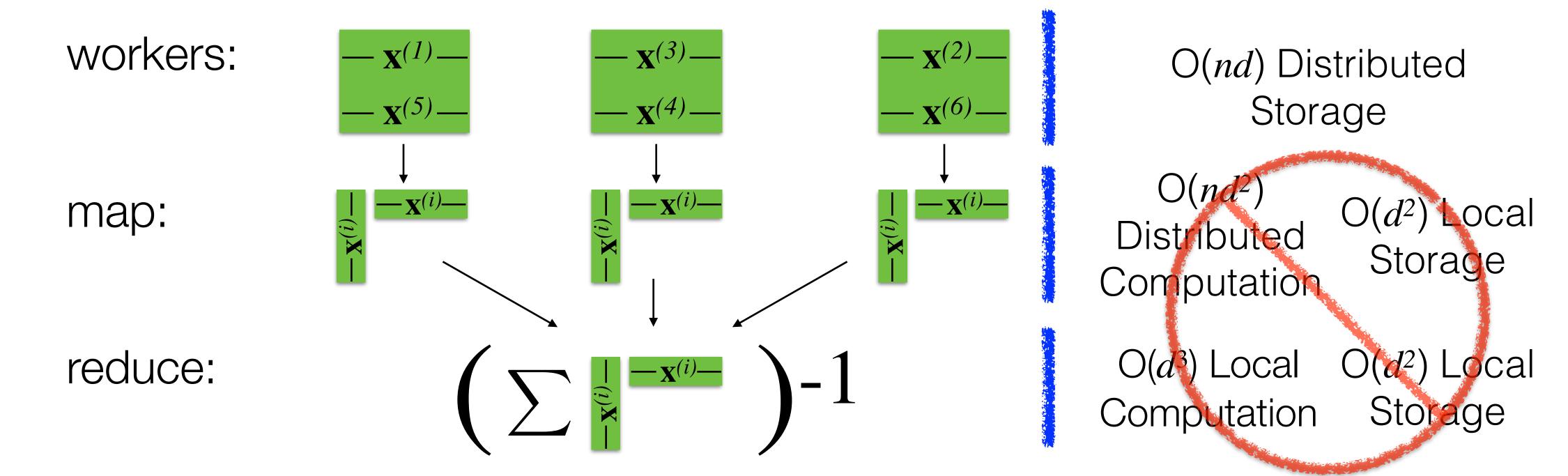


Example: n = 6; 3 workers





Example: n = 6; 3 workers



$$\mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Computation: $O(nd^2 + d^3)$ operations

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

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

Can't easily distribute!

1st Rule of thumb

Computation and storage should be linear (in n, 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

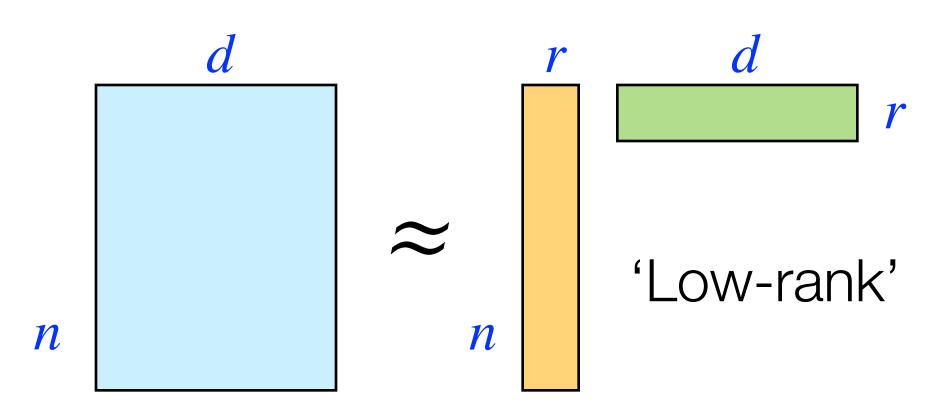
```
dense: 1. 0. 0. 0. 0. 0. 3.

sparse: {
    size: 7
    indices: 0 6
    values: 1. 3.
```

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



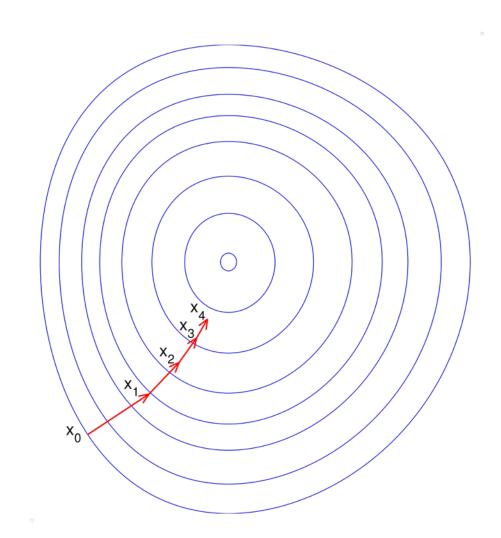
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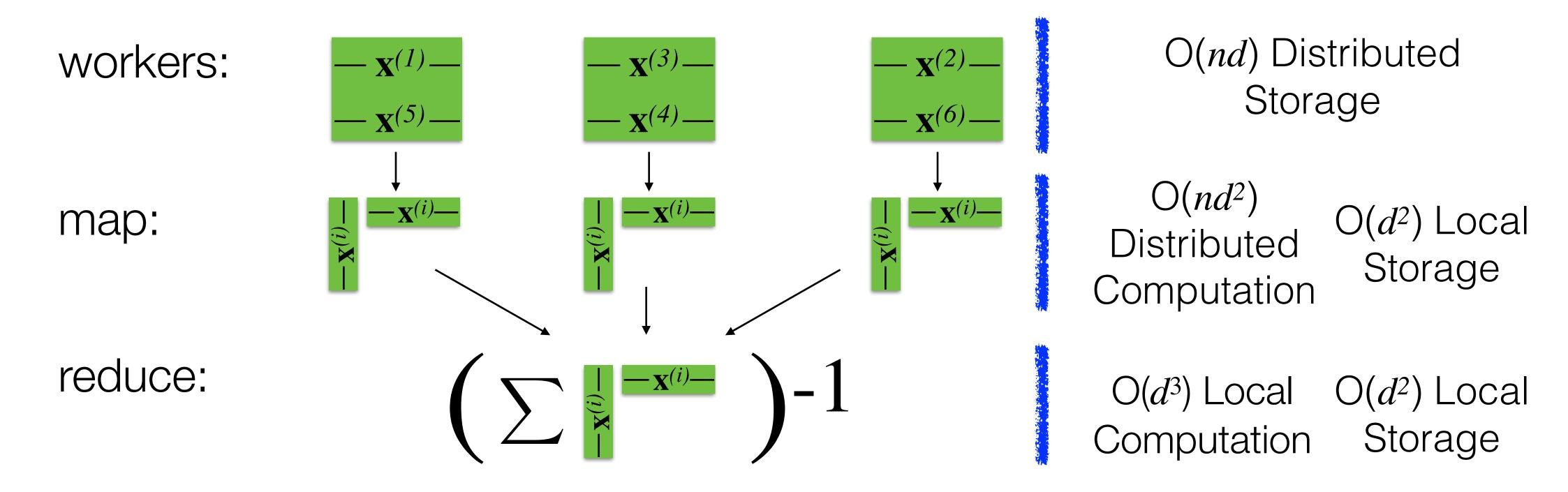
Another idea: Use different algorithms

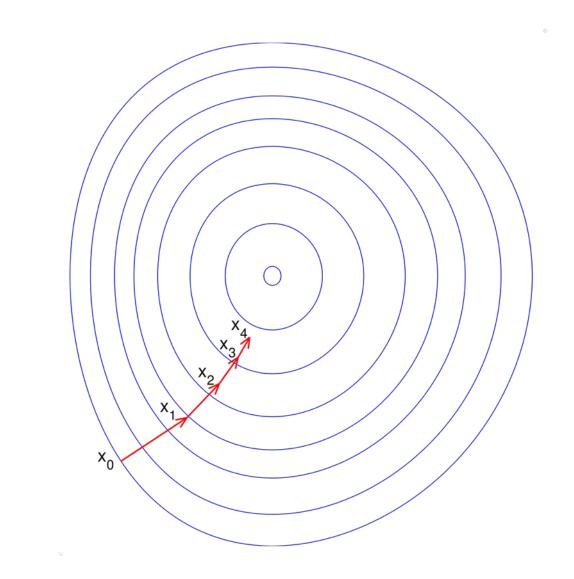
 Gradient descent is an iterative algorithm that requires O(nd) computation and O(d) local storage per iteration



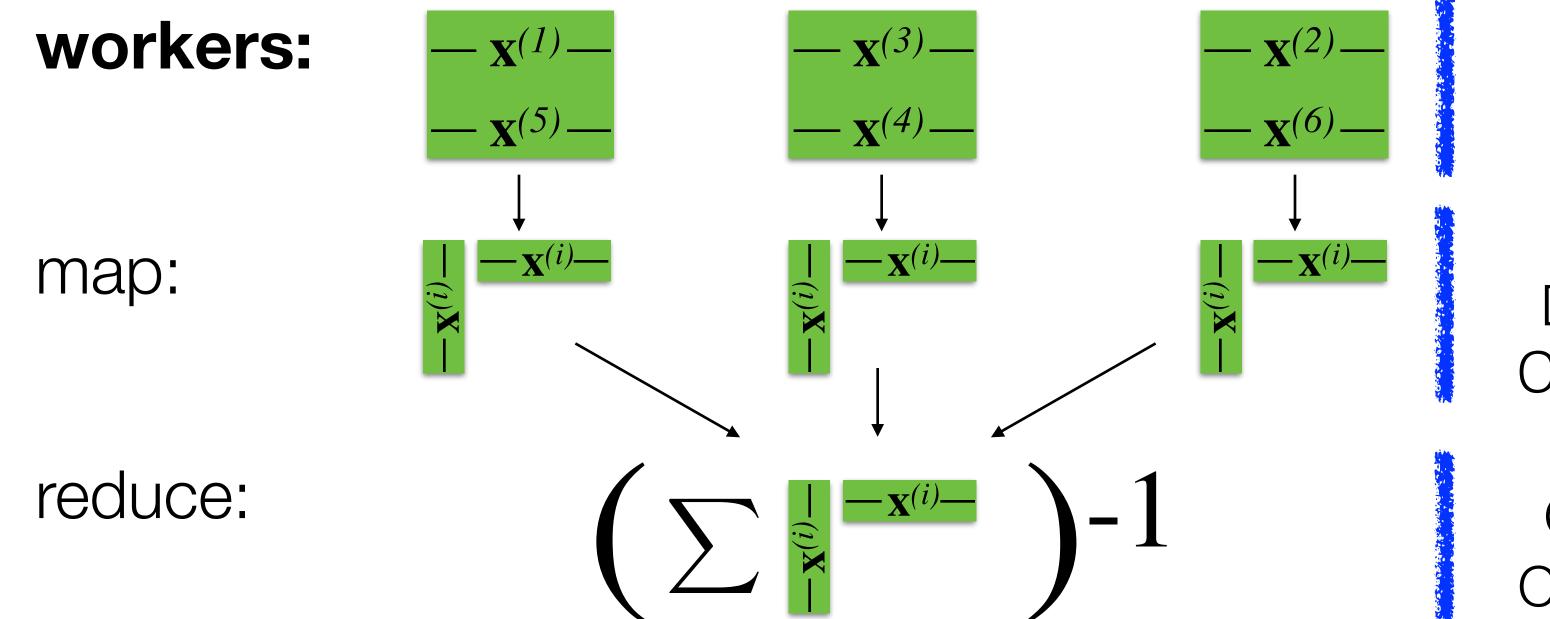
Closed Form Solution for Big n and Big d

Example: n = 6; 3 workers





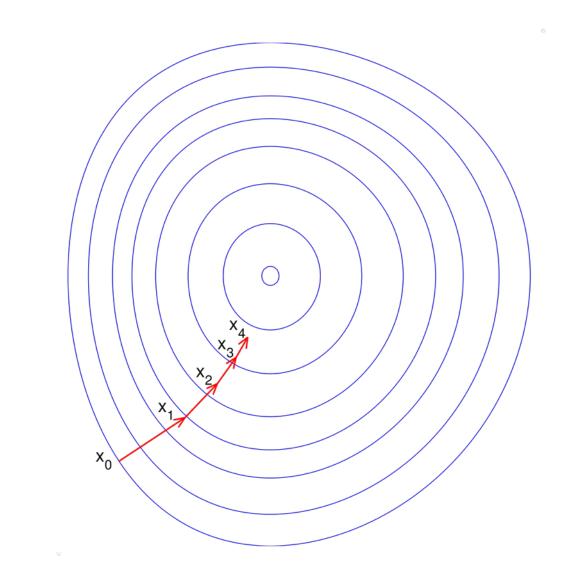
Example: n = 6; 3 workers



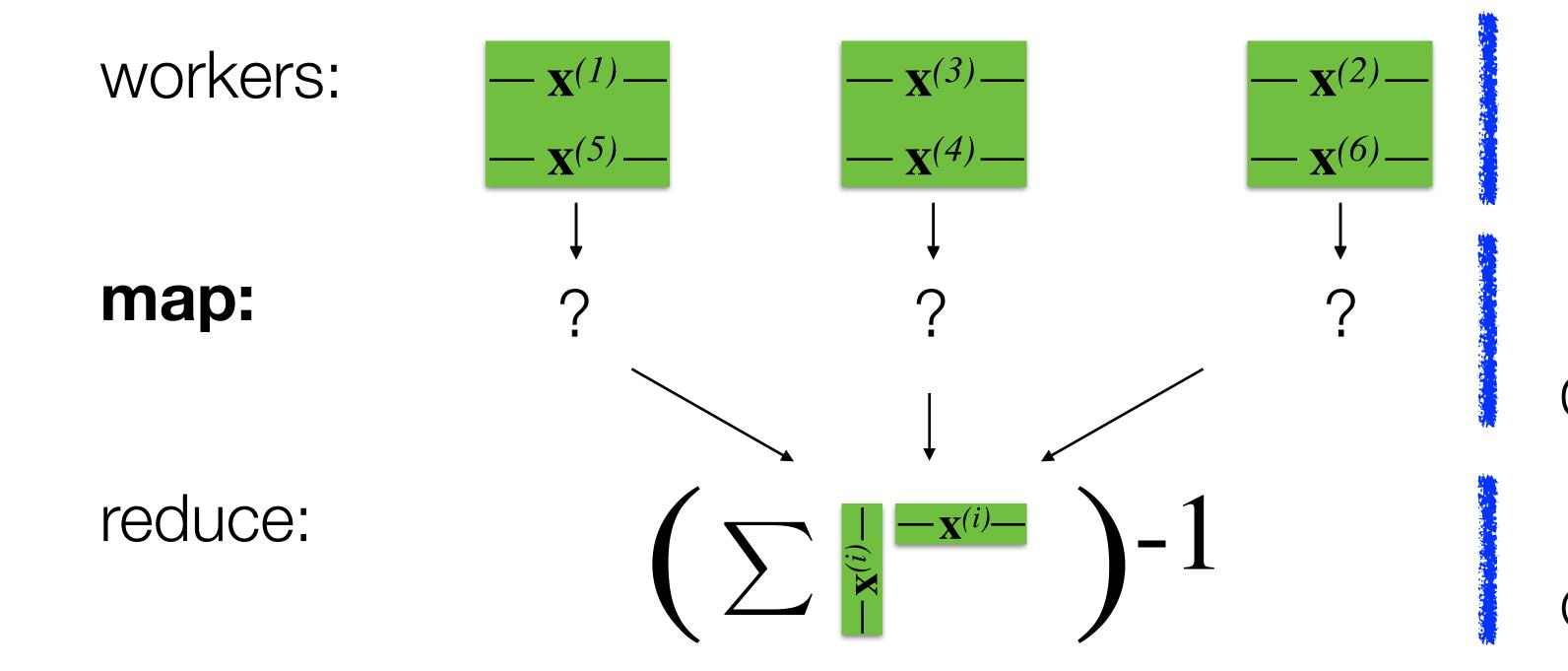
O(nd) Distributed Storage

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

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



Example: n = 6; 3 workers



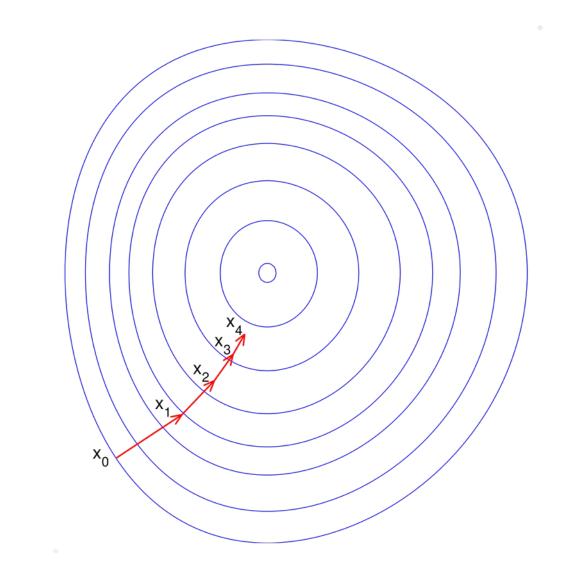
O(nd) Distributed
Storage O(nd) O(nd) O(nd) O(nd)

 $O(nd^2)$ Distributed

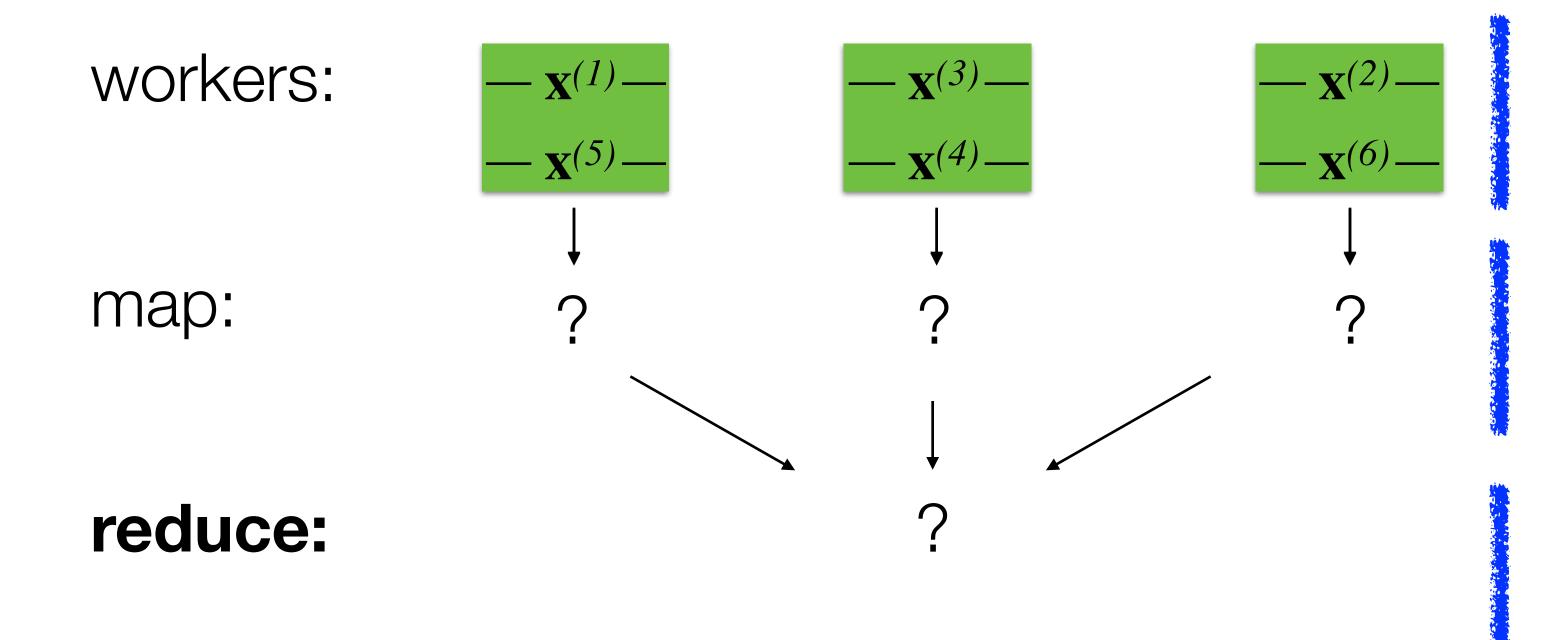
Computation

O(a) $O(d^2)$ Local Storage

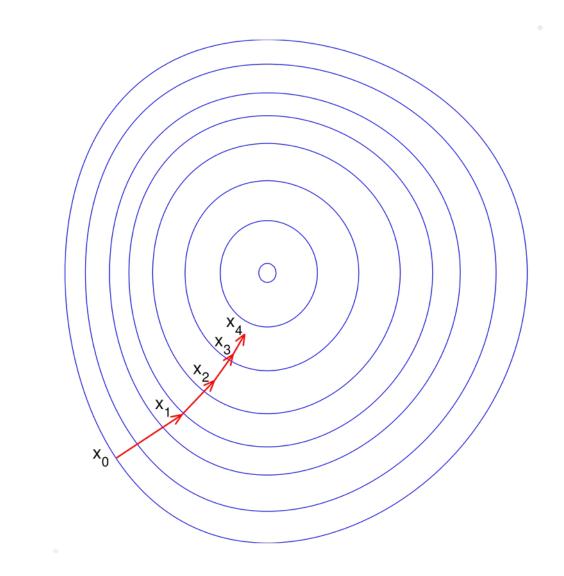
 $O(d^3)$ Local $O(d^2)$ Local Computation Storage



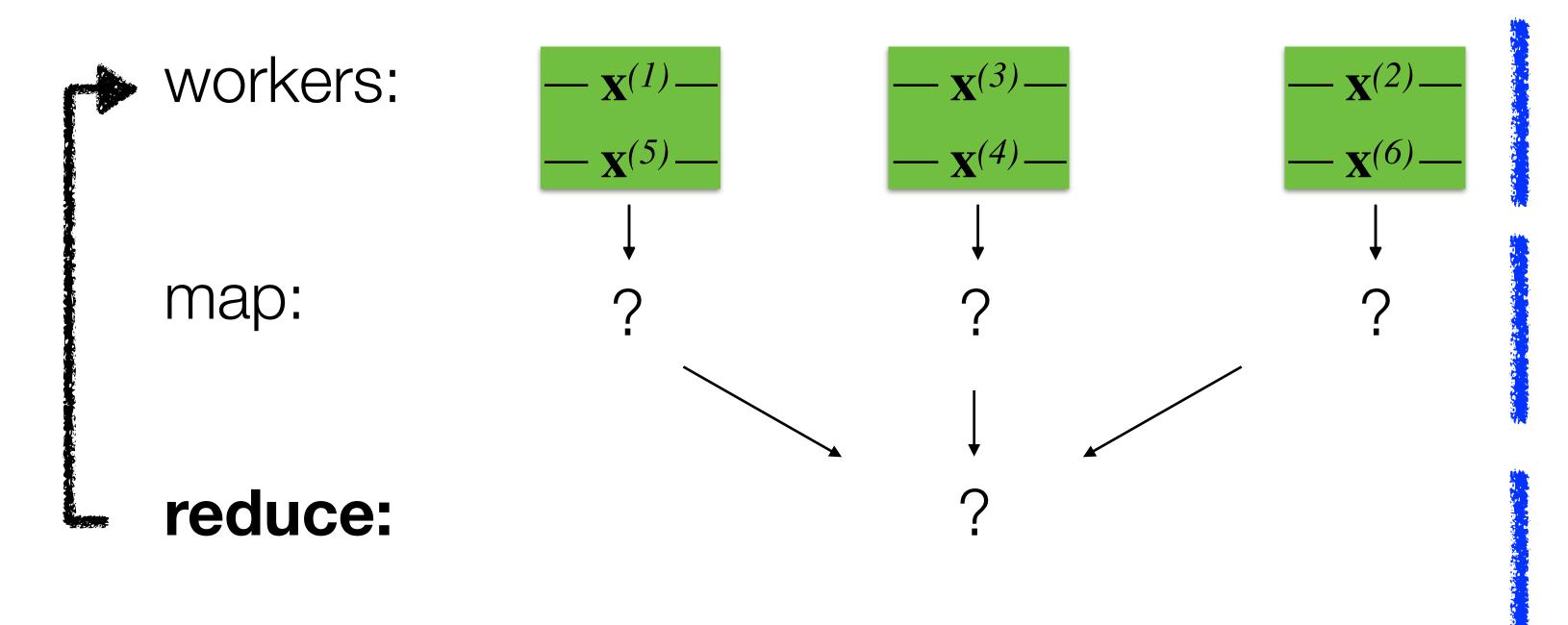
Example: n = 6; 3 workers



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



Example: n = 6; 3 workers



O(nd) Distributed
Storage

O(nd)
O(nd^2)
O(nd^2)
Oistributed
Computation
O(d)
O(d)
O(d^3)
Local
Computation
Storage