Learning Models by Fitting Parameters: Linear and Ridge Regression

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CS5350/6350: Machine Learning

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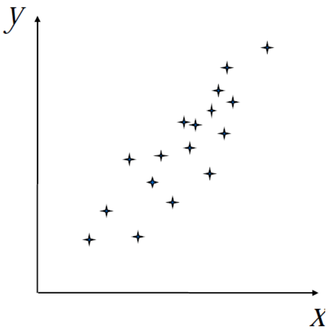
Linear Regression: One-Dimensional Case



- **Given:** a set of N input-response pairs
- The inputs (x) and the responses (y) are one dimensional scalars
- **Goal:** Model the relationship between x and y

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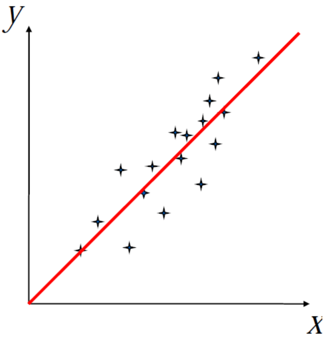

- Let's assume the relationship between x and y is linear

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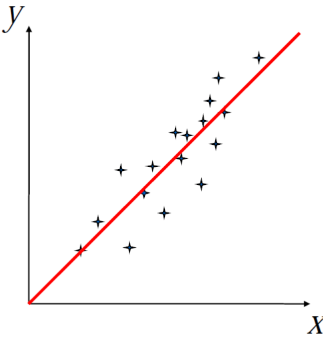

- Let's assume the relationship between x and y is linear
- Linear relationship can be defined by a straight line with *parameter* w
- Equation of the straight line: $y = wx$

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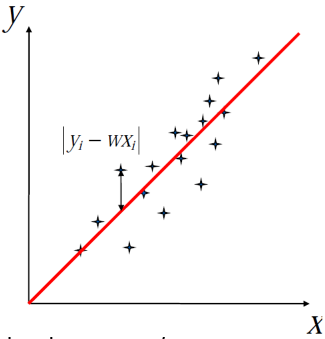

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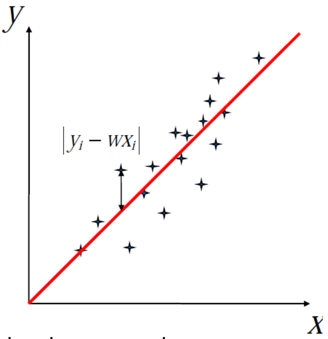

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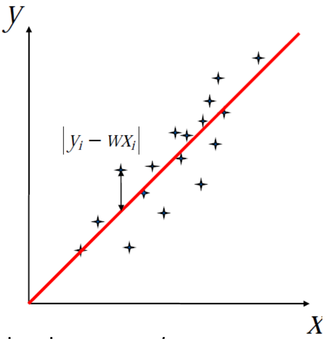

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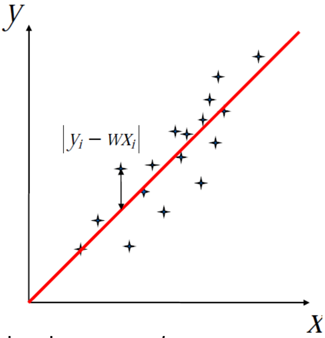

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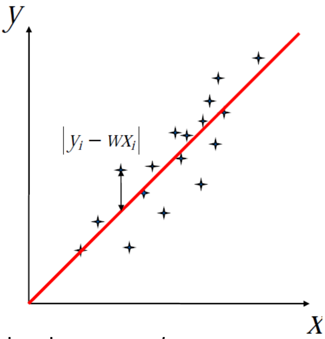

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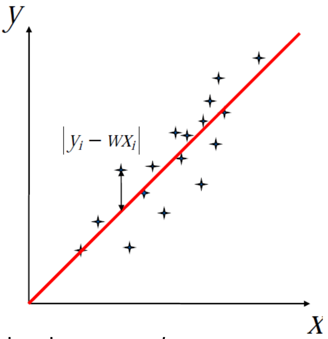

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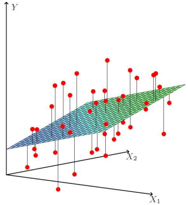
- The best fitting line is defined by w minimizing the total error E
- Just requires a little bit of calculus to find it (take derivative, equate to zero..)

Linear Regression: In Higher Dimensions

- **Analogy to line fitting:** In higher dimensions, we will fit hyperplanes
- For 2-dim. inputs, linear regression fits a 2-dim. plane to the data



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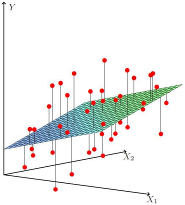

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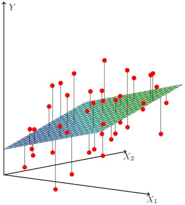

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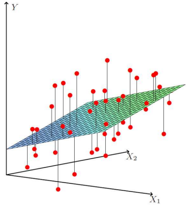

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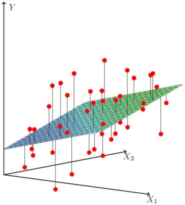

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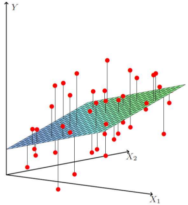

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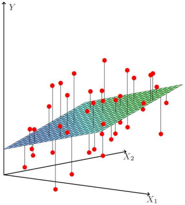

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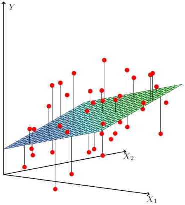

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  - Fitting a D-dimensional hyperplane to the data
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- The hyperplane is defined by parameters $\mathbf{w}$ (a $D \times 1$ weight vector)

Linear Regression: In Higher Dimensions (Formally)

- Given training data $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
- Inputs $\mathbf{x}_i$: D-dimensional vectors ($\mathbb{R}^D$), responses y_i: scalars ($\mathbb{R}$)

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  - Parameters define the mapping from the inputs to responses
- Each ϕ_j is called a basis function
  - Allows change of representation of the input $\mathbf{x}$ (often desired)

Linear Regression: In Higher Dimensions

The linear model:

$$y = b + \sum_{j=1}^{M} w_j \phi_j(\mathbf{x}) = b + \mathbf{w}^T \phi(\mathbf{x})$$

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- $\mathbf{w} = [w_1, \ldots, w_M]$, the **weight vector** (to learn using the training data)

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- **Note:** Nonlinear relationships between $\mathbf{x}$ and y can be modeled using suitably chosen ϕ_j's (more when we cover Kernel Methods)

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- Given training data $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
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- $\mathbf{Y}$: $N \times 1$, $\mathbf{X}$: $N \times (D+1)$, $\mathbf{w}$: $(D+1) \times 1$

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- Following the matrix notation, we can write the above as:

$$E(\mathbf{w}) = \frac{1}{2} (\mathbf{Y} - \mathbf{X}\mathbf{w})^T (\mathbf{Y} - \mathbf{X}\mathbf{w})$$

Linear Regression: Least-Squares Solution

- Taking derivative w.r.t $\mathbf{w}$, and equating to zero, we get

$$\begin{aligned} \nabla E(\mathbf{w}) &= -\mathbf{X}^T(\mathbf{Y} - \mathbf{X}\mathbf{w}) = 0 \\ \Longrightarrow \mathbf{X}^T\mathbf{X}\mathbf{w} &= \mathbf{X}^T\mathbf{Y} \end{aligned}$$

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- **Note:** The same solution holds even if the responses are vector-valued (assume K responses per input)
  - $\mathbf{Y}$ will be an $N \times K$ matrix (assuming K responses per input)
  - $\mathbf{w}$ will be a $D \times K$ matrix (k-th column is the weight vector for the k-th response variable)

Linear Regression: Complexity Control

- We minimized the sum-of-squares objective for linear regression

$$E(\mathbf{w}) = \frac{1}{2}(\mathbf{Y} - \mathbf{X}\mathbf{w})^T(\mathbf{Y} - \mathbf{X}\mathbf{w})$$

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- Penalizing the squared norm $\mathbf{w}^T\mathbf{w}$ is a common choice (called ℓ_2 norm)
$$\mathbf{w}^T\mathbf{w} = \sum_{j=1}^{D} w_j^2$$

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  - Result: The model may lead to overfitting
- Solution: Penalize large values of the parameters/coefficients w_i's
  - Penalizing amounts to doing complexity control (also called regularization)
  - Leads to better generalization
- Penalizing the squared norm $\mathbf{w}^T\mathbf{w}$ is a common choice (called ℓ_2 norm)
$$\mathbf{w}^T\mathbf{w} = \sum_{j=1}^{D} w_j^2$$
- **Note:** other form of penalization are also possible. For example:
  - Sum of absolute values of the coefficients: $\sum_{j=1}^{D} |w_j|$ (called ℓ_1 norm)

Linear Regression: The Regularized Objective Function

- The modified objective becomes

$$E(\mathbf{w}) = \frac{1}{2}(\mathbf{Y} - \mathbf{X}\mathbf{w})^T(\mathbf{Y} - \mathbf{X}\mathbf{w}) + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

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- The hyperparameter λ controls the amount of regularization
- **Important:** It's a standard way to control overfitting in supervised learning
- Common form of a penalized loss function in supervised learning looks like:

$$\boxed{E(\mathbf{w}) = \ell(\mathbf{X}, \mathbf{Y}, \mathbf{w}) + R(\mathbf{w})}$$

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- Regularization is particularly important for small N, large D

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Coming back to the penalized least-squares objective for linear regression

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- Ridge regression also useful when $\mathbf{X}^T\mathbf{X}$ is not invertible
  - Standard least-squares solution $\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ will not be valid
  - Adding the $\lambda\mathbf{I}$ makes $(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})$ invertibe

Linear Regression: Gradient Descent Solution

- Recall: solving for $\mathbf{w}$ requires inverting $D \times D$ matrices $\mathbf{X}^T\mathbf{X}$ or $(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})$
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- How: Using Gradient Descent (GD)
- A *general recipe* for iteratively optimizing similar loss functions
- Gradient Descent rule:
  - Initialize the weight vector $\mathbf{w} = \mathbf{w}^0$
  - Update $\mathbf{w}$ by moving along the direction of negative gradient $-\frac{\partial \mathbf{E}}{\partial \mathbf{w}}$

Linear Regression: Gradient Descent Solution

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Linear Regression: Gradient Descent Solution

- Initialize $\mathbf{w} = \mathbf{w}^0$
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$$\mathbf{w} = \mathbf{w} - \alpha \frac{\partial \mathbf{E}}{\partial \mathbf{w}}$$

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- α is the learning rate
- **Stop:** When some criteria is met (e.g., max. # of iterations), or the rate of decrease of **E** falls below some threshold
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- Note that convergence rate depends on the *error* at each iteration
  - Error over all examples: $\sum_{i=1}^{N} \mathbf{x}_i(\mathbf{w}^T\mathbf{x}_i - y_i)$

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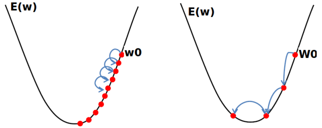

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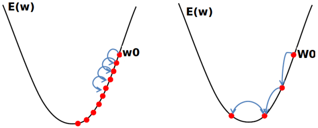

- **Stochastic Gradient Descent (SGD):** Variant of GD which computes the gradient of $E(\mathbf{w})$ w.r.t. a single training example and thus allows updating $\mathbf{w}$ using one example at a time (unlike GD which uses *all the data* to make each update of $\mathbf{w}$). SGD for linear regression looks like:
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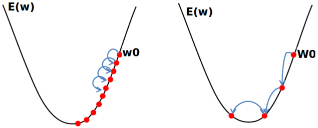

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- Note: SGD is usually more efficient than GD and also converges faster

Next class..

- Linear Classifiers
  - Hyperplane based class separators
  - The Perceptron algorithm
  - Maximum Margin Hyperplanes: Introduction to Support Vector Machines