Linear Models and Learning via Optimization

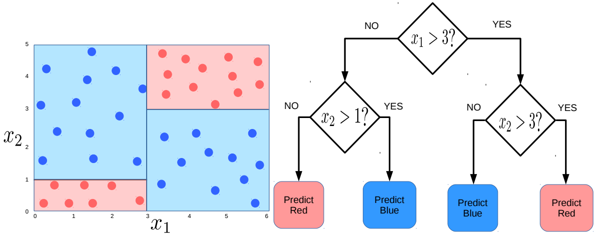
Piyush Rai

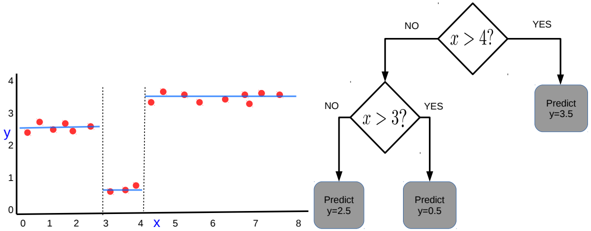
Introduction to Machine Learning (CS771A)

August 9, 2018

Recap

Decision Trees: Learning by asking questions. Ask the "important" questions first!





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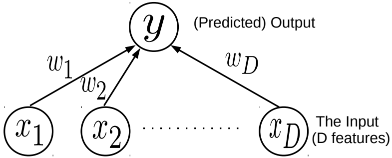

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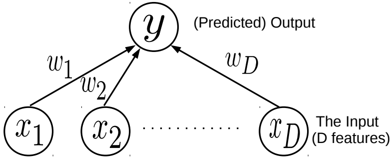

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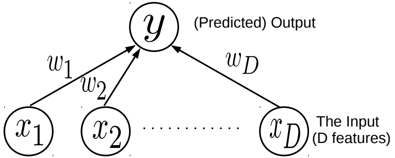

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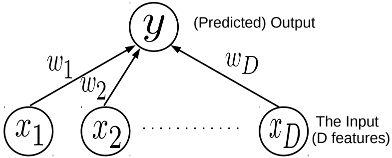

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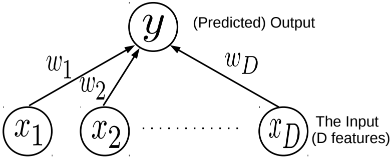

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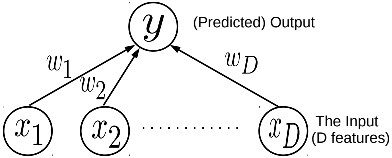

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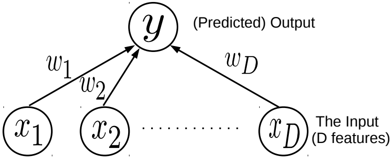

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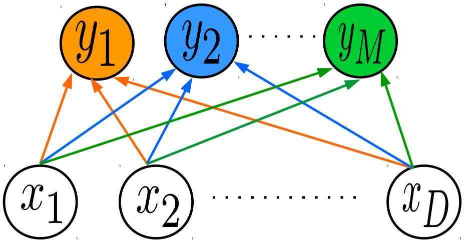
- This basic model can also be used as building blocks in many more complex models

Linear Models for Multi-output Regression

- Can assume each of the M outputs in $\boldsymbol{y} \in \mathbb{R}^M$ to be modeled by a linear model



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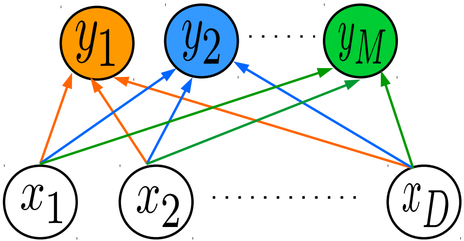

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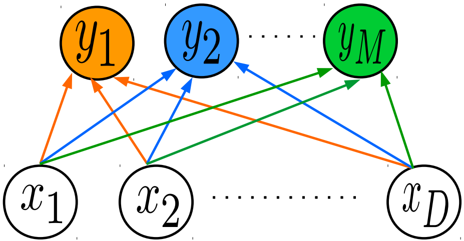

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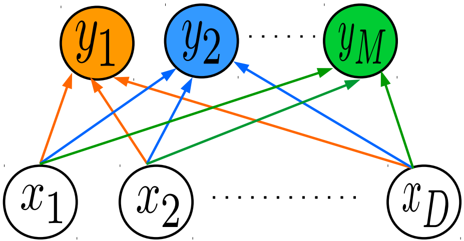

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- $\mathbf{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_M]$ is a $D \times M$ matrix

Linear Models for Binary Classification

- Use the sign of the "score" $\boldsymbol{w}^\top \boldsymbol{x}$ to do predict binary label

$$y = +1 \quad \text{if} \quad \boldsymbol{w}^\top \boldsymbol{x} \geq 0$$
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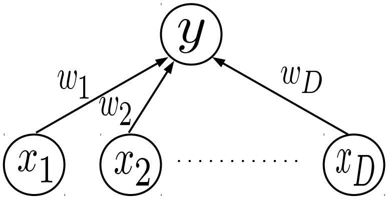

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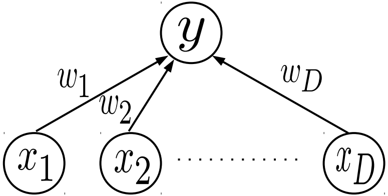

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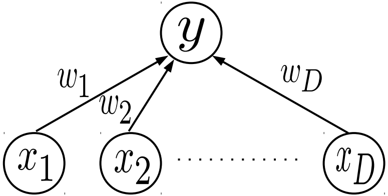

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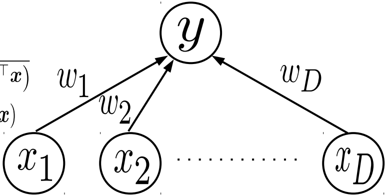
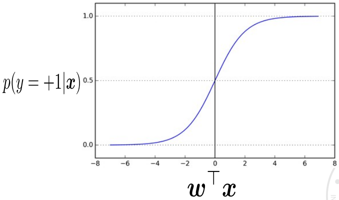
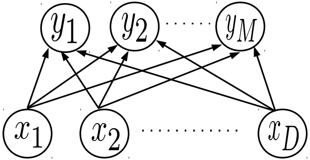
$$p(y = +1|\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^\top \boldsymbol{x})}$$
$$p(y = -1|\boldsymbol{x}) = 1 - p(y = +1|\boldsymbol{x})$$





Linear Models for Multi-class/Multi-label Classification

- Recall that, in multi-class/multi-label classification, $\boldsymbol{y} = [y_1, y_2, \ldots, y_M]$ is a vector of length M



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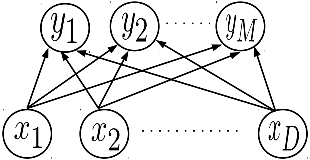

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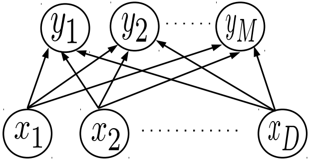

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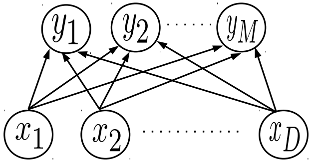

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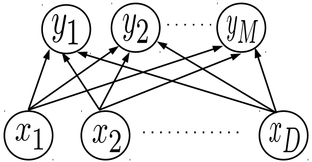

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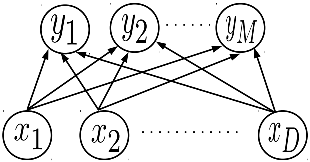

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  - Can use the indices of top few entries in $\boldsymbol{y}$ as the predicted labels in multi-label classification

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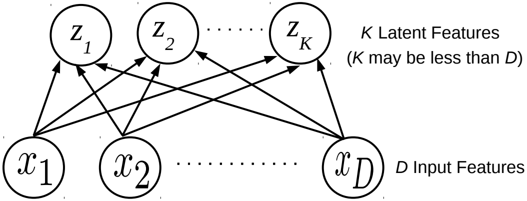
Linear Models for Dimensionality Reduction

- Linear models can be used to reduce data-dimensionality (e.g., Principal Component Analysis)



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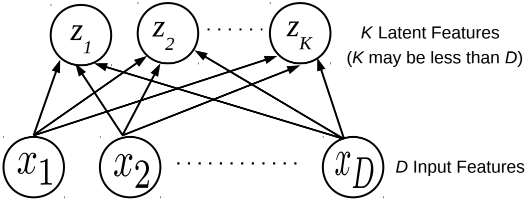

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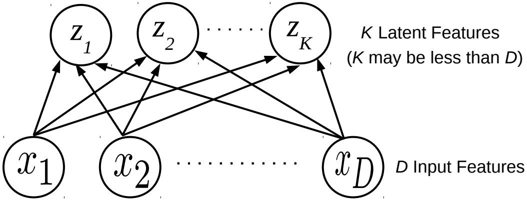

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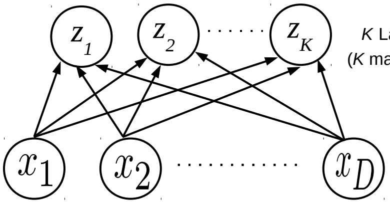

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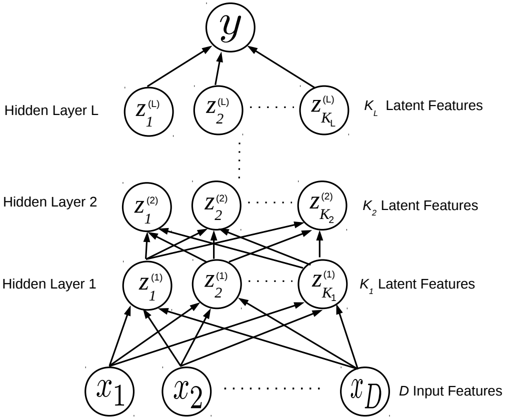
  - An example of an unsupervised learning problem
- Need to learn both $\boldsymbol{z}$ and $\mathbf{W}$ in these problems

Linear Models to construct Deep Neural Networks

- Linear models are used as basic components of deep neural networks (nonlinear models)



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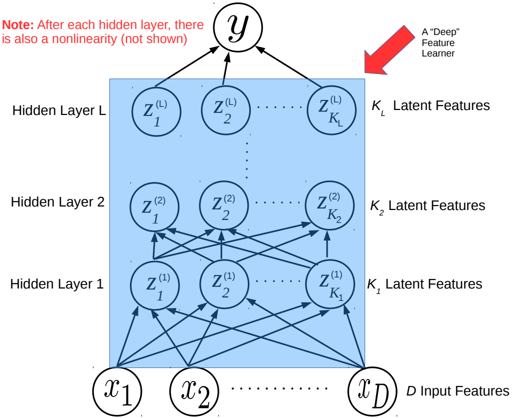

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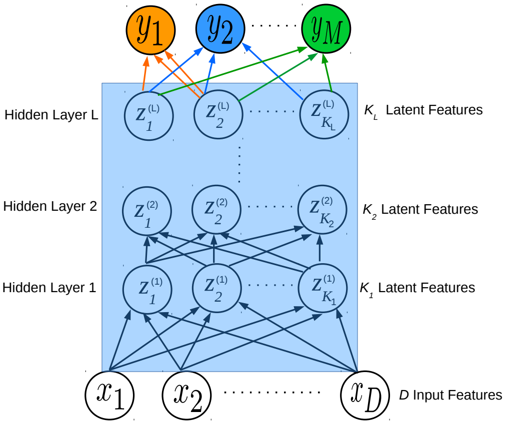

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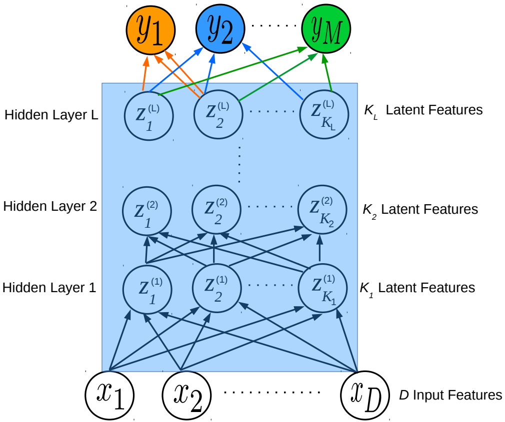
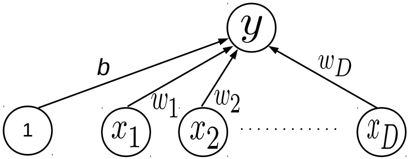


- These can be used for multi-output regression, multi-class/multi-label classification, etc.

Linear Models with Offset (Bias) Parameter

- Some linear models use an additional bias parameter b



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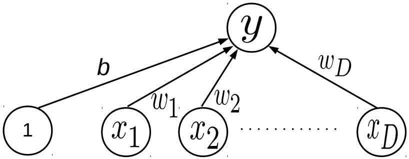

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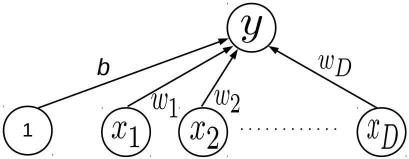

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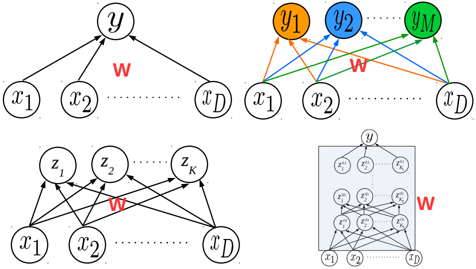
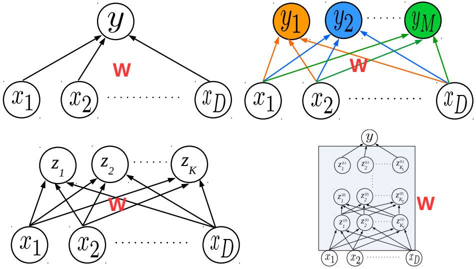
- We will assume the same and omit the explicit bias for simplicity of notation

Learning Linear Models



Linear Models are ubiquitous!

Learning Linear Models



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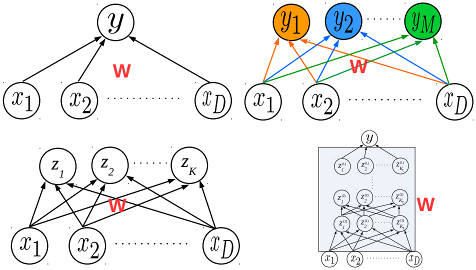

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For linear models, learning = Learning the model parameters (the weights)

We will formulate learning as an optimization problem w.r.t. these parameters

Learning a Linear Model for Regression

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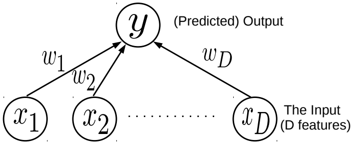

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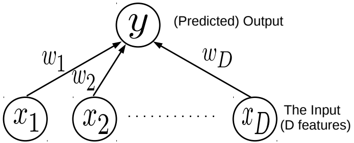

- Suppose we are given regression training data $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$ with $\boldsymbol{x}_n \in \mathbb{R}^D$, and $y_n \in \mathbb{R}$

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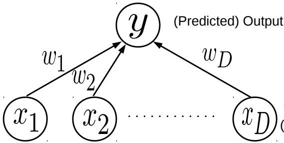

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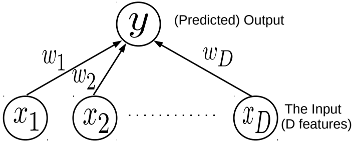

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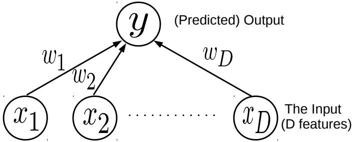

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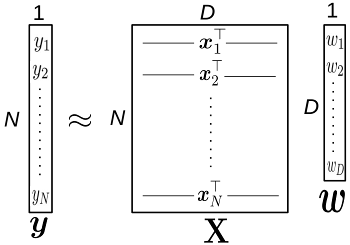
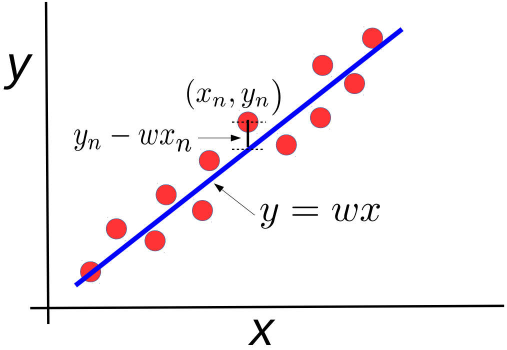


Linear Regression: Pictorially

- With one-dimensional inputs, linear regression would look like



- Error of the model for an example $= y_n - \boldsymbol{w}^\top \boldsymbol{x}_n$ ($= y_n - wx_n$ for scalar input case)

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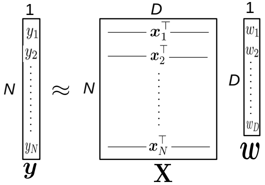

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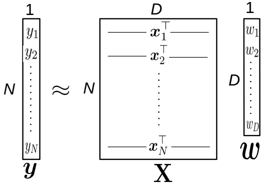

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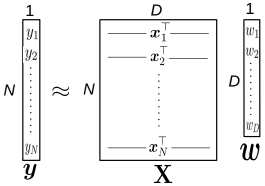

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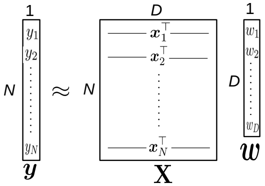

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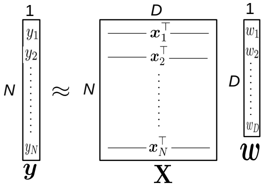

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  - Expensive inversion for large D: Can used iterative optimization techniques (will come to this later)

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- Note that, in this case, regularization also made inversion possible (note the $\lambda \mathbf{I}_D$ term)

How ℓ_2 Regularization Helps Here?

- We saw that ℓ_2 regularization encourages the individual weights in $\boldsymbol{w}$ to be small
- Small weights ensure that the function $y = f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}$ is smooth (i.e., we expect similar $\boldsymbol{x}$'s to have similar y's). Below is an informal justification:
- Consider two points $\boldsymbol{x}_n \in \mathbb{R}^D$ and $\boldsymbol{x}_m \in \mathbb{R}^D$ that are exactly similar in all features except the d-th feature where they differ by a small value, say ϵ
- Assuming a simple/smooth function $f(\boldsymbol{x})$, y_n and y_m should also be close
- However, as per the model $y = f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}$, y_n and y_m will differ by ϵw_d
- Unless we constrain w_d to have a small value, the difference ϵw_d would also be very large (which isn't what we want).
- That's why regularizing (via ℓ_2 regularization) and making the individual components of the weight vector small helps

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  - Note: Since they learn a sparse $\boldsymbol{w}$, ℓ_0 or ℓ_1 regularization is also useful for doing feature selection ($w_d = 0$ means feature d is irrelevant). We will revisit ℓ_1 later to formally see why ℓ_1 gives sparsity

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  - Using ℓ_0 norm encourages very few non-zero entries in $\boldsymbol{w}$ (thereby promoting "sparse" $\boldsymbol{w}$)

$$||\boldsymbol{w}||_0 = \#\text{nnz}(\boldsymbol{w})$$

  - Optimizing with ℓ_0 is difficult (NP-hard problem); can use ℓ_1 norm as an approximation

$$||\boldsymbol{w}||_1 = \sum_{d=1}^{D} |w_d|$$

  - Note: Since they learn a sparse $\boldsymbol{w}$, ℓ_0 or ℓ_1 regularization is also useful for doing feature selection ($w_d = 0$ means feature d is irrelevant). We will revisit ℓ_1 later to formally see why ℓ_1 gives sparsity
- Other techniques for regularization: Early stopping (of training), "dropout", etc (popular in deep neural networks; will revisit these later when discussing deep learning)

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- Such iterative methods for optimizing loss functions are widely used in ML. Will revisit these later

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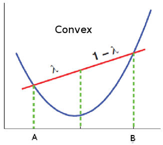

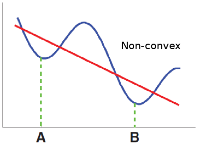

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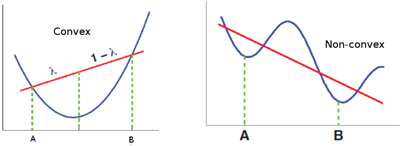

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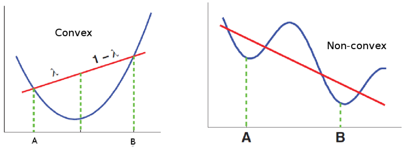

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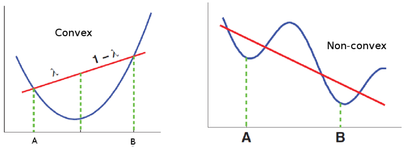

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- For Gradient Descent, the learning rate is important (should not be too large or too small)

Linear Regression as Solving System of Linear Equations

- Solving $\boldsymbol{y} = \mathbf{X}\boldsymbol{w}$ for $\boldsymbol{w}$ is like solving for D unknowns $w_1, \ldots, w_D$ using N equations

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- Thus methods to solve over/underdetermined systems can be used to solve linear regression as well
    - Many of these don't require a matrix inversion (will provide a separate note with details)

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  - Generalized Linear Model $y_n = g(\boldsymbol{w}^\top \boldsymbol{x}_n)$ when response y_n is not real-valued but binary/categorical/count, etc, and g is a "link function"

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$$\hat{f} = \arg\min_{f} \mathcal{L}_{reg}(f) = \arg\min_{f} \sum_{n=1}^{N} \ell(y_n, f(\boldsymbol{x}_n)) + \lambda R(f)$$

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General Supervised Learning as Optimization

- We saw that regularized least squares regression required solving

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- As we'll see later, different supervised learning problems differ in the choice of f, $R(.)$, and ℓ

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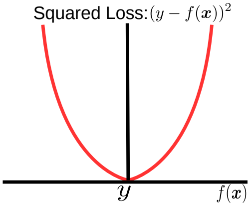

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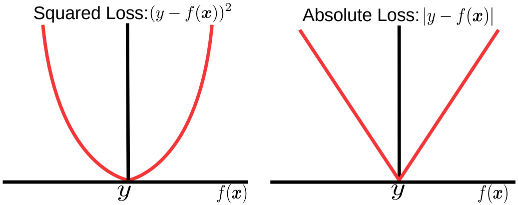

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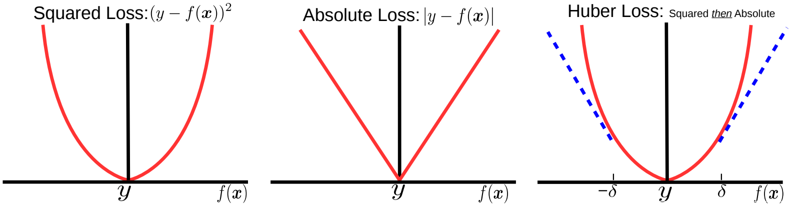

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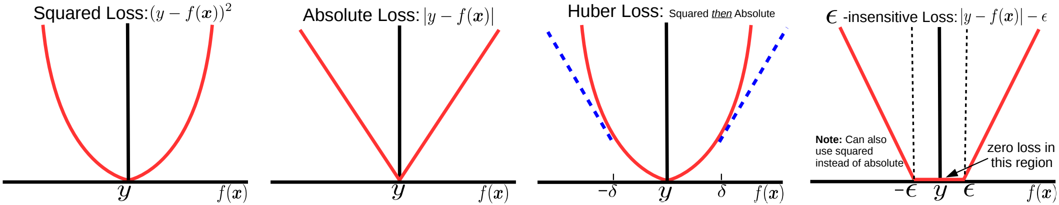

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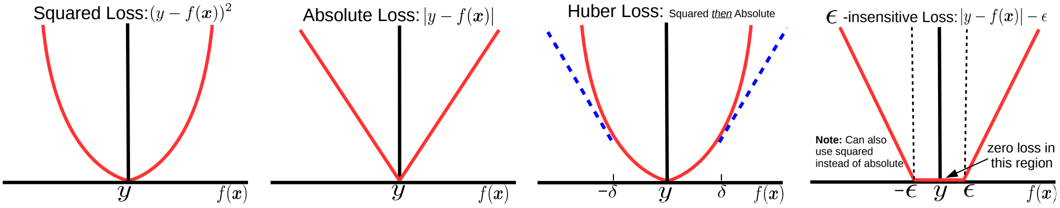

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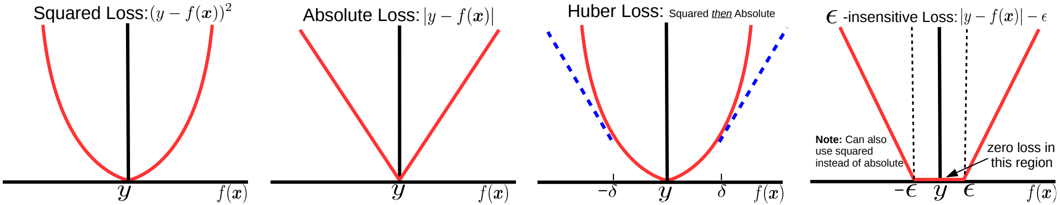

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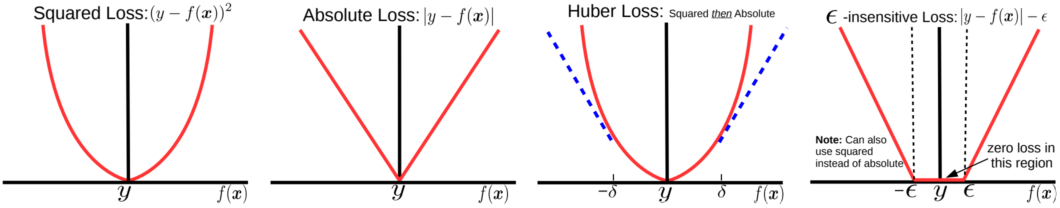

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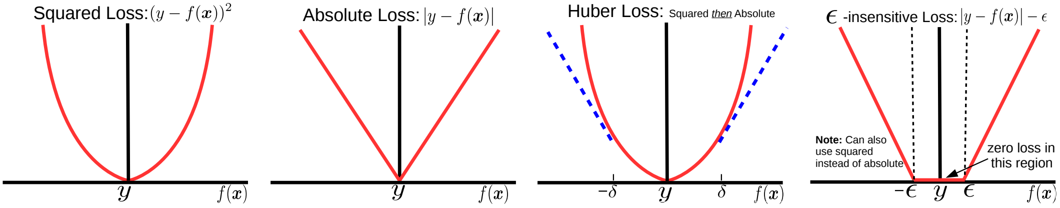

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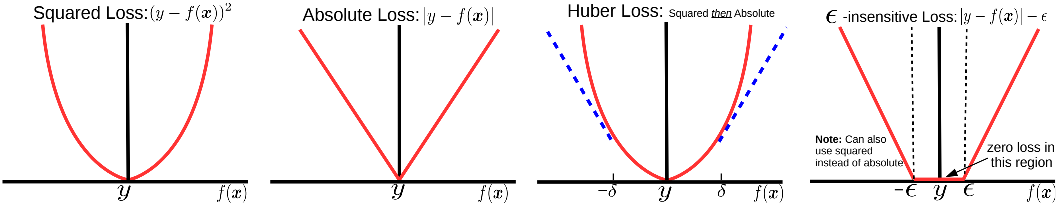

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- Will revisit many of these aspects when we talk about optimization techniques for ML

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- In this case both f and $\mathbf{Z}$ need to be learned. Typically learned via alternating optimization