Linear Models and Learning via Optimization

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Introduction to Machine Learning (CS771A)

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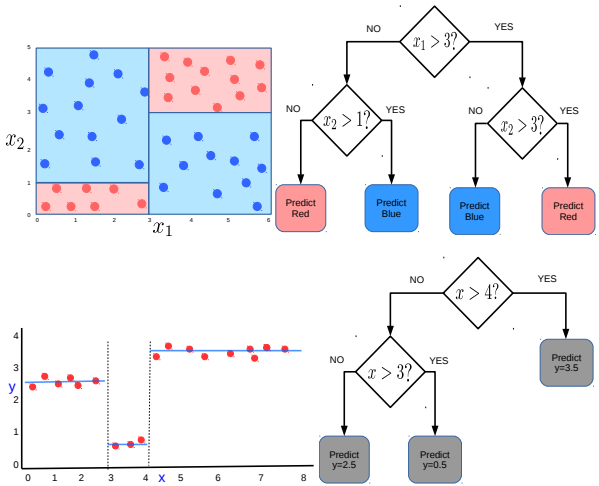
Recap

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

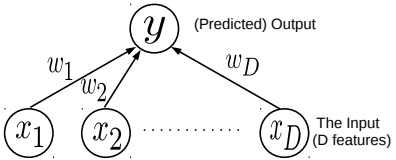


Linear Models

Linear Models

- Consider learning to map an input $\boldsymbol{x} \in \mathbb{R}^D$ to its output y (say real-valued)
- Assume the output to be a linear weighted combination of the D input features

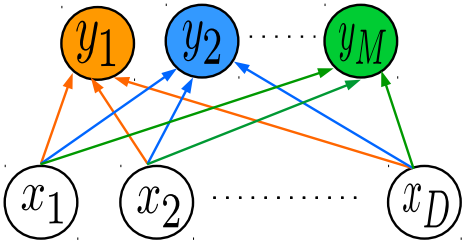
$$y = \sum_{d=1}^{D} w_d x_d = \boldsymbol{w}^\top \boldsymbol{x}$$



- This is an example of a linear model with D parameters $\boldsymbol{w} = [w_1, w_2, \ldots, w_D]$
- Inspired by **linear models of neurons**
- $\boldsymbol{w} \in \mathbb{R}^D$ is also known as the weight vector
- Here w_d denotes how important the d-th input feature is for predicting y
- The above is basically a linear model for simple regression (single, real-valued output y)
- 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

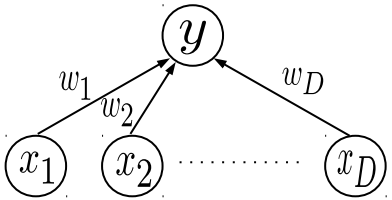


- Each output y_m $(m = 1, \ldots, M)$ modeled by a weight vector $\boldsymbol{w}_m \in \mathbb{R}^D$: $y_m = \boldsymbol{w}_m^\top \boldsymbol{x}$
- The entire model for all M outputs can be represented as $\boldsymbol{y} = \mathbf{W}^\top \boldsymbol{x}$
- $\mathbf{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_M]$ is a $D \times M$ matrix

Linear Models for Binary Classification

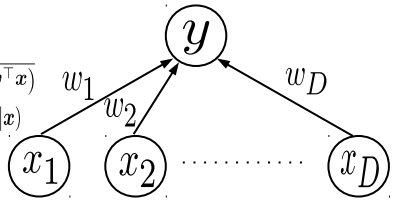
- Use the sign of the "score" $\boldsymbol{w}^\top \boldsymbol{x}$ to do predict binary label

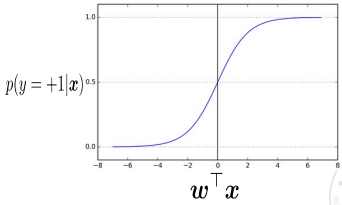
$$y = +1 \quad \text{if} \quad \boldsymbol{w}^\top \boldsymbol{x} \geq 0$$
$$y = -1 \quad \text{if} \quad \boldsymbol{w}^\top \boldsymbol{x} < 0$$
$$y = \text{sign}(\boldsymbol{w}^\top \boldsymbol{x})$$



- If desired, can turn the score $\boldsymbol{w}^\top \boldsymbol{x}$ into the probability of the label being $+1$ (logistic regression)

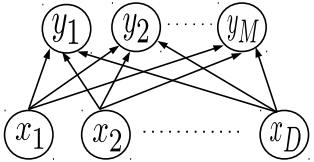
$$p(y = +1|\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^\top \boldsymbol{x})}$$
$$p(y = -1|\boldsymbol{x}) = 1 - p(y = +1|\boldsymbol{x})$$





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

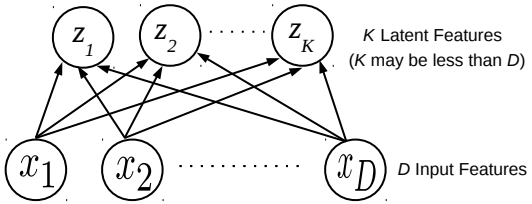


- Just like multi-output regression, each component y_m of $\boldsymbol{y}$ can be modeled by a weight vector $\boldsymbol{w}_m$
- Need a way to convert $\boldsymbol{y} \in \mathbb{R}^M$ to one-hot (for multi-class)/binary vector (for multi-label)
- Note: In some cases, the score need not be converted, e.g.,
  - Can use the index of largest entry in $\boldsymbol{y}$ as the predicted class in multi-class classification

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

Linear Models for Dimensionality Reduction

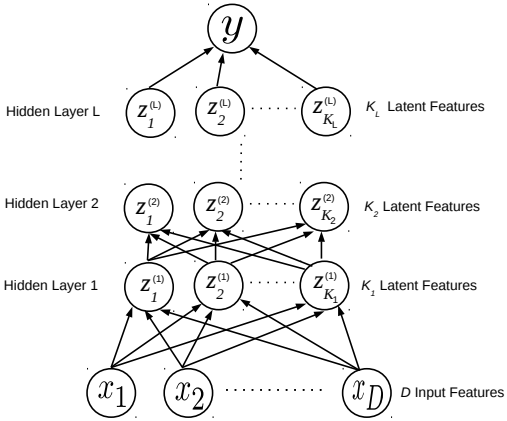
- Linear models can be used to reduce data-dimensionality (e.g., Principal Component Analysis)



- Note that it looks similar to multi-output regression but the output vector $\boldsymbol{z}$ is latent
  - 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

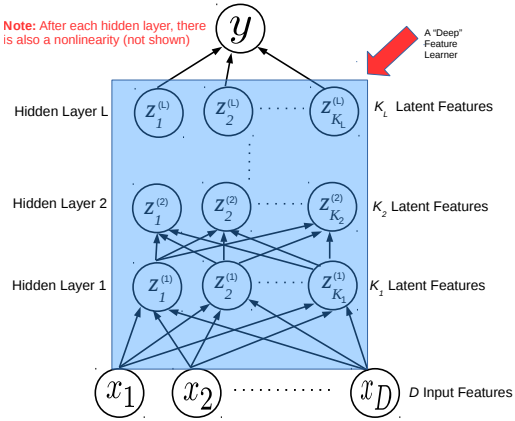
- Linear models are used as basic components of deep neural networks (nonlinear models)



- Each hidden layer has a learned **latent features** based representation of the original input $\boldsymbol{x}$

Linear Models to construct Deep Neural Networks

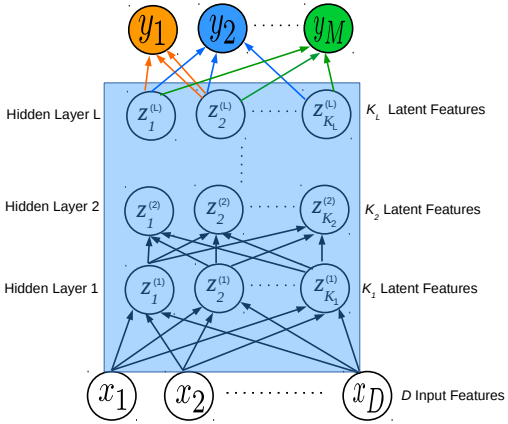
- Linear models are used as basic components of deep neural networks (nonlinear models)



- Each hidden layer has a learned **latent features** based representation of the original input $\boldsymbol{x}$

Linear Models to construct Deep Neural Networks

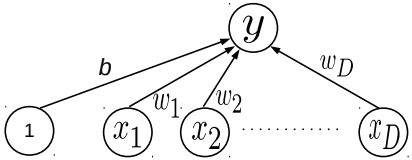
- Can even construct multiple-output versions of deep neural network



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

Linear Models with Offset (Bias) Parameter

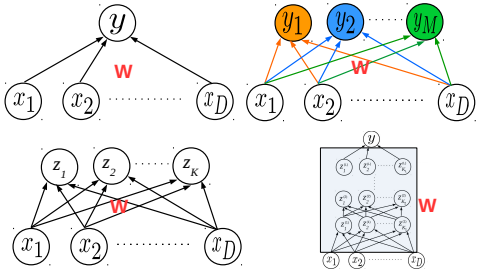
- Some linear models use an additional bias parameter b



$$y = \sum_{d=1}^{D} w_d x_d + b = \boldsymbol{w}^\top \boldsymbol{x} + b$$

- Can append a constant feature "1" for each input and rewrite as $y = \boldsymbol{w}^\top \boldsymbol{x}$, with $\boldsymbol{x}, \boldsymbol{w} \in \mathbb{R}^{D+1}$
- We will assume the same and omit the explicit bias for simplicity of notation

Learning Linear Models



Linear Models are ubiquitous!

How do we learn them from data?

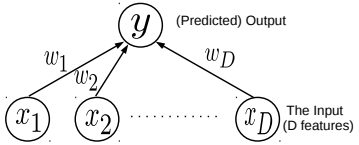
For linear models, learning = Learning the model parameters (the weights)

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

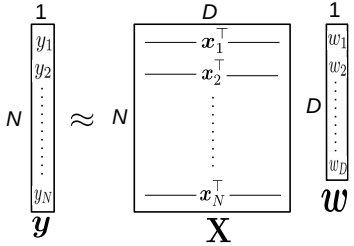
Learning a Linear Model for Regression

- Let's focus on learning the simplest linear model for now: Linear Regression

$$y = \sum_{d=1}^{D} w_d x_d = \boldsymbol{w}^\top \boldsymbol{x}$$

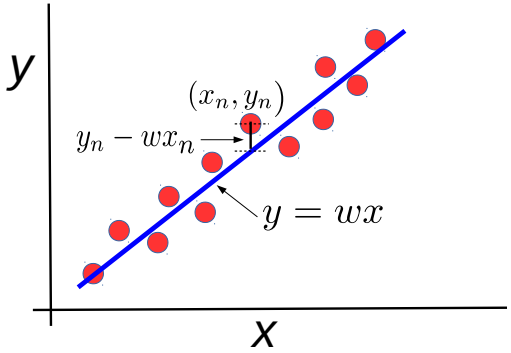


- Suppose we are given regression training data $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^{N}$ with $\boldsymbol{x}_n \in \mathbb{R}^D$, and $y_n \in \mathbb{R}$
- Let's model the training data using $\boldsymbol{w}$ and assume $y_n \approx \boldsymbol{w}^\top \boldsymbol{x}_n$, $\forall n$ (equivalently $\boldsymbol{y} \approx \mathbf{X}\boldsymbol{w}$)



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)

Linear Regression

- Define the total error or "loss" on the training data, when using $\boldsymbol{w}$ as our model, as

$$\mathcal{L}(\boldsymbol{w}) = \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

- Note: Squared loss chosen for simplicity. Can define other type of losses too (more on this later)
- The best $\boldsymbol{w}$ will be the one that minimizes the above error (requires optimization w.r.t. $\boldsymbol{w}$)

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

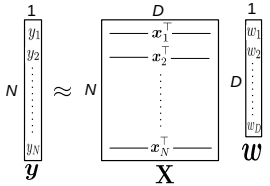
- This is known as "least squares" linear regression (Gauss/Legendre, early 18th century)
- Taking derivative (gradient) of $\mathcal{L}(\boldsymbol{w})$ w.r.t. $\boldsymbol{w}$ and setting to zero

$$\sum_{n=1}^{N} 2(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n) \frac{\partial}{\partial \boldsymbol{w}} (y_n - \boldsymbol{x}_n^\top \boldsymbol{w}) = 0 \quad \Rightarrow \quad \sum_{n=1}^{N} \boldsymbol{x}_n (y_n - \boldsymbol{x}_n^\top \boldsymbol{w}) = 0$$

- Simplifying further, we get a closed form solution for $\boldsymbol{w} \in \mathbb{R}^D$

$$\boldsymbol{w} = (\sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^\top)^{-1} \sum_{n=1}^{N} y_n \boldsymbol{x}_n = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y}$$

Linear Regression



- Consider the closed form solution we obtained for linear regression based on least squares

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

- The above closed form solution is nice but has some issues
  - The $D \times D$ matrix $\mathbf{X}^\top \mathbf{X}$ may not be invertible
  - Based solely on minimizing the training error $\sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 \Rightarrow$ can overfit the training data
  - Expensive inversion for large D: Can used iterative optimization techniques (will come to this later)

Regularized Linear Regression (a.k.a. Ridge Regression)

- Consider regularized loss: Training error + ℓ_2-squared norm of $\boldsymbol{w}$, i.e., $||\boldsymbol{w}||_2^2 = \boldsymbol{w}^\top \boldsymbol{w} = \sum_{d=1}^{D} w_d^2$

$$\mathcal{L}_{reg}(\boldsymbol{w}) = \left[\sum_{n=1}^{N}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \frac{\lambda}{2}\boldsymbol{w}^\top \boldsymbol{w}\right]$$

- Minimizing the above objective w.r.t. $\boldsymbol{w}$ does two things
  - Keeps the training error small
  - Keeps the ℓ_2 norm of $\boldsymbol{w}$ small (and thus also the individual components of $\boldsymbol{w}$): **Regularization**
- There is a trade-off between the two terms: The regularization hyperparam $\lambda > 0$ controls it
  - Very small λ means almost no regularization (can overfit)
  - Very large λ means very high regularization (can underfit - high training error)
  - Can use cross-validation to choose the "right" λ
- The solution to the above optimization problem is: $\boldsymbol{w} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1}\mathbf{X}^\top \boldsymbol{y}$
- 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

Regularization: Some Comments

- Many ways to regularize ML models (for linear as well as other models)
- Some are based on adding a norm of $\boldsymbol{w}$ to the loss function (as we already saw)
  - Using ℓ_2 norm in the loss function promotes the individual entries $\boldsymbol{w}$ to be small (we saw that)
  - 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)

Linear/Ridge Regression via Gradient Descent

- Both least squares regression and ridge regression require matrix inversion

$$\text{Least Squares} \quad \boldsymbol{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y}, \quad \text{Ridge} \quad \boldsymbol{w} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \mathbf{X}^\top \boldsymbol{y}$$

- Can be computationally expensive when D is very large
- A faster way is to use iterative optimization, such as batch or stochastic gradient descent
- A basic batch gradient-descent based procedure looks like
  - Start with an initial value of $\boldsymbol{w} = \boldsymbol{w}^{(0)}$
  - Update $\boldsymbol{w}$ by moving along the gradient of the loss function $\mathcal{L}$

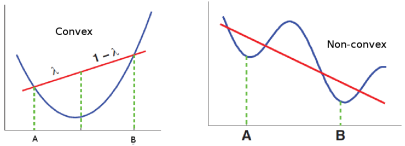
$$\boldsymbol{w}^{(t)} = \boldsymbol{w}^{(t-1)} - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{w}}\bigg|_{\boldsymbol{w}=\boldsymbol{w}^{(t-1)}} \qquad \text{where } \eta \text{ is the learning rate}$$

  - Repeat until converge
- For least squares, the gradient is $\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = -\sum_{n=1}^{N} \boldsymbol{x}_n (y_n - \boldsymbol{x}_n^\top \boldsymbol{w})$ (no matrix inversion involved)
- Such iterative methods for optimizing loss functions are widely used in ML. Will revisit these later

Linear Regression via Gradient-based Methods: Some Notes

We will revisit gradient based methods later but a few things to keep in mind

- Gradient Descent guaranteed to converge to a local minima
- Gradient Descent converges to global minima if the function is convex



- A function is convex if second derivative is non-negative everywhere (for scalar functions) or if Hessian is positive semi-definite (for vector-valued functions). For a convex function, every local minima is also a global minima.
- Note: The squared loss function in linear regression is convex
  - With ℓ_2 regularizer, it becomes strictly convex (single global minima)
- 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

$$\begin{aligned} y_1 &= x_{11}w_1 + x_{12}w_2 + \ldots + x_{1D}w_D \\ y_2 &= x_{21}w_1 + x_{22}w_2 + \ldots + x_{2D}w_D \\ &\vdots \\ y_N &= x_{N1}w_1 + x_{N2}w_2 + \ldots + x_{ND}w_D \end{aligned}$$

- Can therefore view the linear regression problem as a system of linear equations
- However, in linear regression, we would rarely have $N = D$, but $N > D$ or $D > N$
- $N > D$ case is an overdetermined system of linear equations (# equations $>$ # unknowns)
- $D > N$ case is an underdetermined system of linear equations (# unknowns $>$ # equations)
- 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)

Linear Regression: Some Other Comments

- A simple and interpretable method. Very widely used.
- Least squares and ridge regression are one of the very few ML problems with closed form solutions

$$\text{Least Squares} \quad \boldsymbol{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y}, \quad \text{Ridge} \quad \boldsymbol{w} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \mathbf{X}^\top \boldsymbol{y}$$

- Many ML problems can be easily reduced to the form $\boldsymbol{y} = \mathbf{X}\boldsymbol{w}$ or $\mathbf{Y} = \mathbf{X}\mathbf{W}$
- Equivalence to over/underdetermined system of linear equations enables us to use efficient solvers (a lot of work in the numerical linear algebra community to scale up linear systems solvers)
  - **An interesting bit:** Note that $\boldsymbol{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y} \Rightarrow \mathbf{A}\boldsymbol{w} = \boldsymbol{b}$ where $\mathbf{A} = \mathbf{X}^\top \mathbf{X}$ and $\boldsymbol{b} = \mathbf{X}^\top \boldsymbol{y}$
  - Using the above relation, can solve for $\boldsymbol{w}$ by solving $\mathbf{A}\boldsymbol{w} = \boldsymbol{b}$. A standard linear system with D equations and D unknowns; can be solved using efficient linear systems solvers.
- The basic (regularized) linear regression can also be easily extended to
  - Nonlinear Regression $y_n \approx \boldsymbol{w}^\top \phi(\boldsymbol{x}_n)$ by replacing the original feature vector $\boldsymbol{x}_n$ by a nonlinear transformation $\phi(\boldsymbol{x}_n)$ (where ϕ may be pre-defined or itself learned)
  - 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"

General Supervised Learning as Optimization

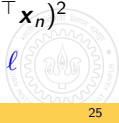
- We saw that regularized least squares regression required solving

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \mathcal{L}_{reg}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}} \left[\sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \frac{\lambda}{2} \boldsymbol{w}^\top \boldsymbol{w} \right]$$

- This is essentially the training loss (called "empirical loss"), plus the regularization term
- In general, for supervised learning, the goal is to learn a function f, s.t. $f(\boldsymbol{x}_n) \approx y_n, \forall n$
- Moreover, we also want to have a simple f, i.e., have some regularization
- Therefore, learning the best f amounts to solving the following optimization problem

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

  where $\ell(y_n, f(\boldsymbol{x}_n))$ measures the model f's training loss on $(\boldsymbol{x}_n, y_n)$ and $R(f)$ is a regularizer
- For least squares regression, $f(\boldsymbol{x}_n) = \boldsymbol{w}^\top \boldsymbol{x}$, and $R(f) = \boldsymbol{w}^\top \boldsymbol{w}$, and $\ell(y_n, f(\boldsymbol{x}_n)) = (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$
- As we'll see later, different supervised learning problems differ in the choice of f, $R(.)$, and ℓ



General Unsupervised Learning as Optimization

- Can we formulate unsupervised learning problems as optimization problems? Yes, of course! :-)
- Consider an unsupervised learning problem with N inputs $\mathbf{X} = \{\boldsymbol{x}_n\}_{n=1}^N$
- Unsupervised, so no labels. Suppose we are interested in learning a new representation $\mathbf{Z} = \{\boldsymbol{z}_n\}_{n=1}^N$
- Assume a function f that models the relationship between $\boldsymbol{x}_n$ and $\boldsymbol{z}_n$

$$\boldsymbol{x}_n \approx f(\boldsymbol{z}_n) \quad \forall n$$

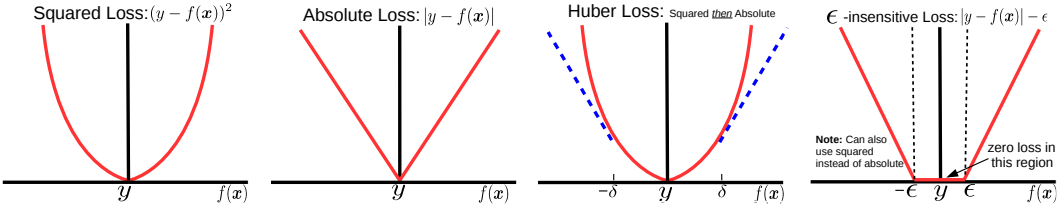
- In this case, we can define a loss function $\ell(\mathbf{x}_n, f(\boldsymbol{z}_n))$ that measures how well f can "reconstruct" the original $\boldsymbol{x}_n$ from its new representation $\boldsymbol{z}_n$
- This generic unsup. learning problem can thus be written as the following optimization problem

$$\hat{f} = \arg\min_{f,\mathbf{Z}} \sum_{n=1}^{N} \ell(\mathbf{x}_n, f(\boldsymbol{z}_n)) + \lambda R(f, \mathbf{Z})$$

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

A Brief Detour: Some Loss Functions

- Some popular loss functions for regression problems[1]



- Absolute/Huber loss preferred if there are outliers in the data
  - Less affected by large errors $|y - f(x)|$ as compared to the squared loss
- Overall objective function = loss func + some regularizer (e.g., ℓ_2, ℓ_1), as we saw for ridge reg.
- Some objectives easy to optimize (convex and differentiable), some not so (e.g., non-differentiable)
- Will revisit many of these aspects when we talk about optimization techniques for ML

[1] will look at loss functions for classification later when discussing classification in detail