Fitting Linear Models, Regularization (revisited) & Cross Validation

Slides by:

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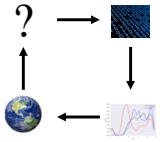
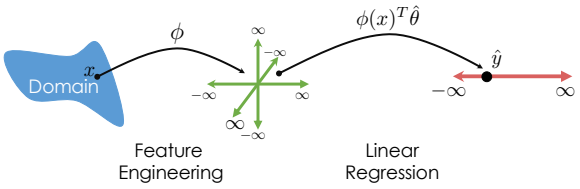


Previously

Feature Engineering and Linear Regression



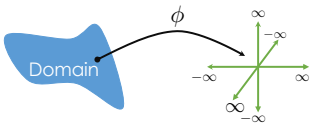
Recap: *Feature Engineering*

- Linear models with feature functions:

$$f_\theta(x) = \sum_{j=1}^{d} \theta_j \phi_j(x)$$

- Feature Functions: $\phi : \mathcal{X} \to \mathbb{R}^d$

Notation: Computer scientist / ML researchers tend to you d (dimensions) and statisticians will use p (parameters).



- **One-hot encoding:** *Categorical Data*

state
NY
WA
CA

AL	...	CA	...	NY	...	WA	...	WY
0	...	0	...	1	...	0	...	0
0	...	0	...	0	...	1	...	0
0	...	1	...	0	...	0	...	0

- **Bag-of-words & N-gram:** *Text Data*

"Learning about machine learning is fun."

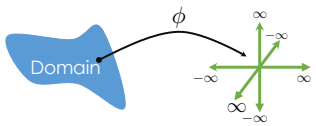
aardvark	...	fun	...	learning	machine	...	zyzzyva
0	0	1	...	2	1	...	0

Vector

- **Custom Features:** *Domain Knowledge*

$$\phi(\text{lat}, \text{lon}, \text{amount}) = \frac{\text{amount}}{\textbf{Stores}[\textbf{ZipCode}[\text{lat}, \text{lon}]]}$$

The Feature Matrix Φ



X DataFrame

uid	age	state	hasBought	review
0	32	NY	True	"Meh."
42	50	WA	True	"Worked out of the box ..."
57	16	CA	NULL	"Hella tofs lit..."

ϕ

$\Phi \in \mathbb{R}^{n \times d}$

AK	...	NY	...	WY	age	hasBought	hasBought missing
0	...	1	...	0	32	1	0
0	...	0	...	0	50	1	0
0	...	0	...	0	16	0	1

Entirely **Quantitative** Values

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uid	age	state	hasBought	review
0	32	NY	True	"Meh."
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0	...	0	...	0	16	0	1

Entirely **Quantitative** Values

Another quick note on confusing notation.

In many textbooks and even in the class notes and discussion you will see:

$$X \in \mathbb{R}^{n \times d} \quad \text{and} \quad \hat{\theta} = \left(X^T X\right)^{-1} X^T Y$$

In this case we are assuming ***X*** is the transformed data **Φ**. This can be easier to read but hides the feature transformation process.

Capital Letter: *Matrix or Random Variable?*
- Both tend to be capitalized
- Unfortunately, there is no common convention … you will have to use context.

The Feature Matrix Φ

AK	...	NY	...	WY	age	hasBought	hasBought missing
0	...	1	...	0	32	1	0
0	...	0	...	0	50	1	0
0	...	0	...	0	16	0	1

Entirely **Quantitative** Values

$\Phi \in \mathbb{R}^{n \times d} = \phi\left[X\right] =$ DataFrame

$$\begin{bmatrix} \phi\left(x^{(1)}\right) \\ \phi\left(x^{(2)}\right) \\ \cdots \\ \phi\left(x^{(n)}\right) \end{bmatrix}$$

n, d

Rows of the **Φ** matrix correspond to records.

Columns of the **Φ** matrix correspond to features.

Confusing notation!

The Feature Matrix Φ

AK	...	NY	...	WY	age	hasBought	hasBought missing
0	...	1	...	0	32	1	0
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$\Phi \in \mathbb{R}^{n \times d} = \phi\left[X\right] =$ DataFrame

$$\begin{bmatrix} \phi\left(X_{1,\bullet}\right) \\ \phi\left(X_{2,\bullet}\right) \\ \cdots \\ \phi\left(X_{n,\bullet}\right) \end{bmatrix}$$

n, d

Rows of the **Φ** matrix correspond to records.

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Notation Guide

$A_{i,\bullet}$: row i of matrix A.

$A_{\bullet,j}$: column j of matrix A.

Making Predictions

$\Phi \in \mathbb{R}^{n \times d} = \phi\left[X\right] =$ DataFrame

$$\begin{bmatrix} \phi\left(X_{1,\bullet}\right) \\ \phi\left(X_{2,\bullet}\right) \\ \cdots \\ \phi\left(X_{n,\bullet}\right) \end{bmatrix}$$

n, d

Rows of the **Φ** matrix correspond to records.

Columns of the **Φ** matrix correspond to features.

Prediction

$$\hat{Y} = f_{\hat{\theta}}(X) = \Phi\hat{\theta} = \begin{bmatrix} \phi\left(X_{1,\bullet}\right) \\ \phi\left(X_{2,\bullet}\right) \\ \cdots \\ \phi\left(X_{n,\bullet}\right) \end{bmatrix} \begin{bmatrix} \hat{\theta} \end{bmatrix} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \cdots \\ \hat{y}^{(n)} \end{bmatrix}$$

n, d

Normal Equations

- Solution to the least squares model:

$$\hat{\theta} = \arg\min \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{d} \theta_j \phi_j(x_i) \right)^2$$

- Given by the normal equation:

$$\hat{\theta} = \left(\Phi^T \Phi\right)^{-1} \Phi^T Y$$

- **You should know this!**
- You do not need to know the calculus based derivation.
- **You should know the geometric derivation …**

Geometric Derivation: **Not Bonus Material**

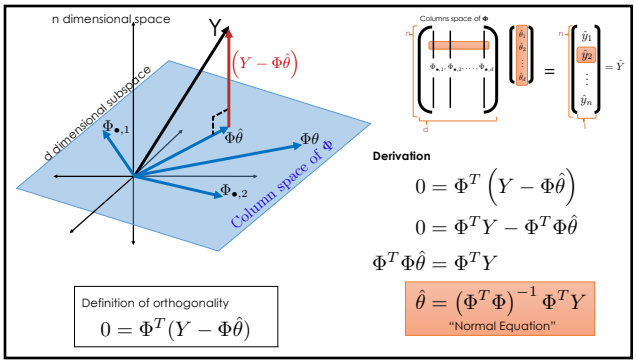
We decided you that this is too exciting to not know.

- Examine the column spaces:

Columns space of **Φ**

$$\begin{bmatrix} \Phi_{\bullet,1}, \Phi_{\bullet,2}, \ldots, \Phi_{\bullet,d} \end{bmatrix} \begin{bmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \\ \vdots \\ \hat{\theta}_d \end{bmatrix} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \hat{Y}$$

n, d, 1



The Normal Equation $\hat{\theta} = (\Phi^T\Phi)^{-1}\Phi^T Y$

$$\hat{\theta}_{d} = \left(\underset{d}{\overset{n}{\Phi^T}}\ \underset{}{\overset{d}{\Phi}}\right)^{-1}\left(\underset{d}{\overset{n}{\Phi^T}}\ \underset{}{\overset{1}{Y}}\right)$$

Note: For inverse to exist **Φ** needs to be full column rank.
→ cannot have co-linear features
This can be addressed by adding regularization …

In practice we will use regression software (e.g., scikit-learn) to estimate θ

Least Squares Regression in Practice

- Use optimized software packages
  - Address numerical issues with matrix inversion
- Incorporate some form of regularization
  - Address issues of collinearity
  - Produce more robust models
- We will be using scikit-learn:
  - http://scikit-learn.org/stable/modules/linear_model.html
  - See Homework 6 for details!

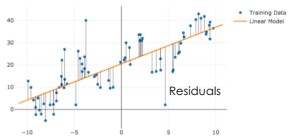
Scikit Learn Models

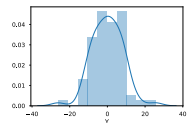
- Scikit Learn has a wide range of models
- Many of the models follow a common pattern:

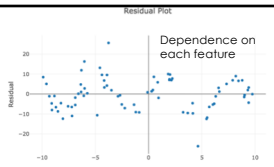
Ordinary Least Squares Regression

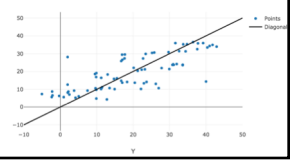
```
from sklearn import linear_model
f = linear_model.LinearRegression(fit_intercept=True)
f.fit(train_data[['X']], train_data['Y'])
Yhat = f.predict(test_data[['X']])
```

Diagnosing Fit → The Residuals





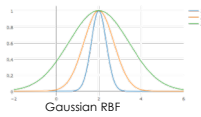


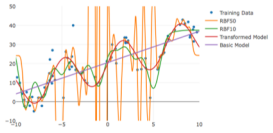


Notebook Demo

- **Generic Features:** *increase model expressivity*
  - **Gaussian Radial Basis Functions:**

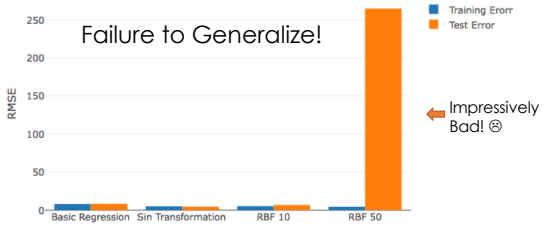
$$\phi_{\lambda_i,\mu_i}(x) = \exp\left(-\frac{||x-\mu_i||_2^2}{\lambda_i}\right)$$





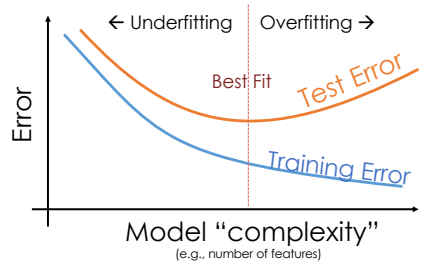
Training Error

Training vs **Test** Error



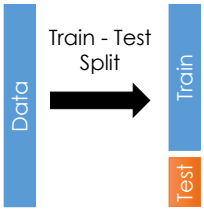
Training vs **Test** Error

Training error typically *under estimates* **test error.**



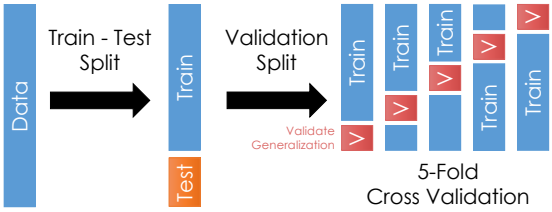
Generalization: *The Train-Test Split*

- **Training Data:** used to fit model
- **Test Data:** check generalization error
- How to split?
  - Randomly, Temporally, Geo…
  - Depends on application (usually randomly)
- What size? (90%-10%)
  - Larger training set → more complex models
  - Larger test set → better estimate of generalization error
  - Typically between 75%-25% and 90%-10%



You can only use the test dataset once after deciding on the model.

Generalization: *Validation Split*



*Cross validation **simulates multiple train test-splits** on the training data.*

Recipe for Successful Generalization

1. Split your data into **training** and **test** sets (90%, 10%)
2. Use **only the training data** when designing, training, and tuning the model
   - Use **cross validation** to test *generalization* during this phase
   - **Do not look at the test data**
3. Commit to your final model and train once more using **only the training data.**
4. Test the final model using the **test data.** If accuracy is not acceptable return to (2). (*Get more test data if possible.*)
5. Train **on all available data** and ship it!

Returning to Regularization

Regularization

Parametrically Controlling the *Model Complexity*

Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that:

f_θ is not too "complicated"

Can we make this more formal?

Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that:

$\text{Complexity}(f_\theta) \leq \beta$

Regularization Parameter

How do we define this?

Idealized Notion of Complexity

$$\text{Complexity}(f_\theta) \leq \beta$$

- Focus on complexity of **linear models:**
  - Number and kinds of features
- Ideal definition:

$$\mathbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right]$$

Number of non-zero parameters

- Why?

Ideal "Regularization"

Find the best value of θ which uses fewer than β features.

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \textbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

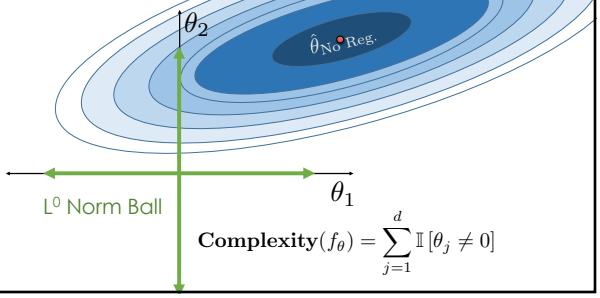
Such that:

Need an approximation!

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Combinatorial search problem → NP-hard to solve in general.

Norm Balls



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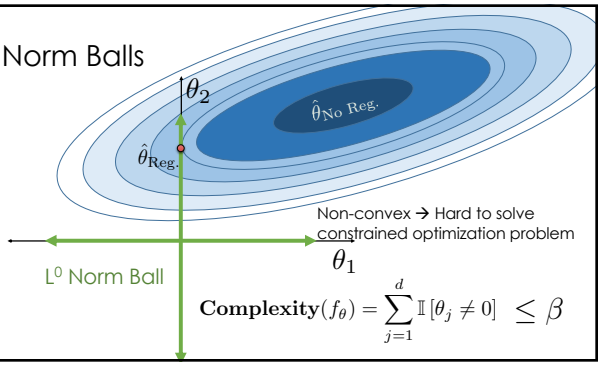
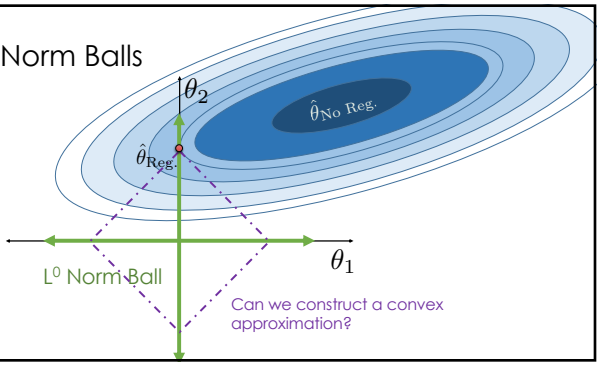


Non-convex → Hard to solve constrained optimization problem

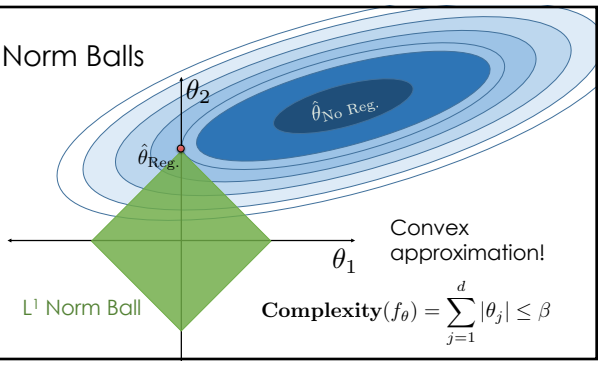
$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Norm Balls



Can we construct a convex approximation?

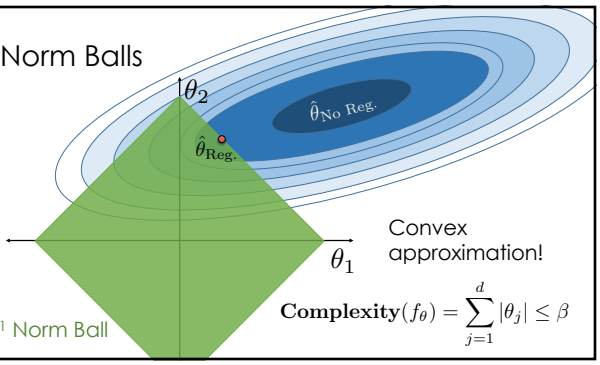
Norm Balls



Convex approximation!

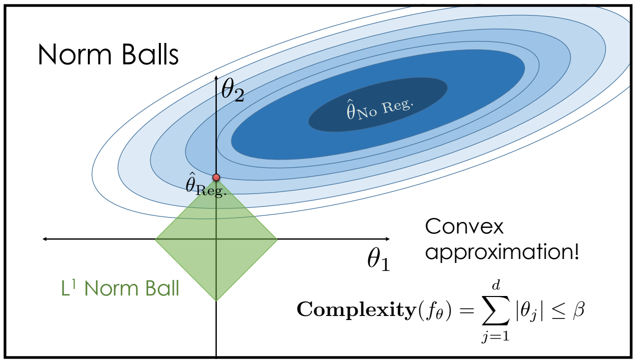
$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$

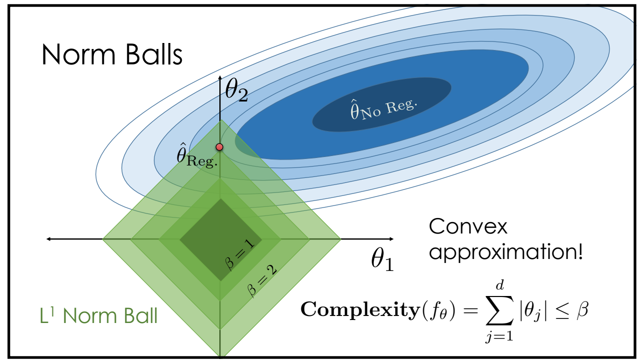
Norm Balls

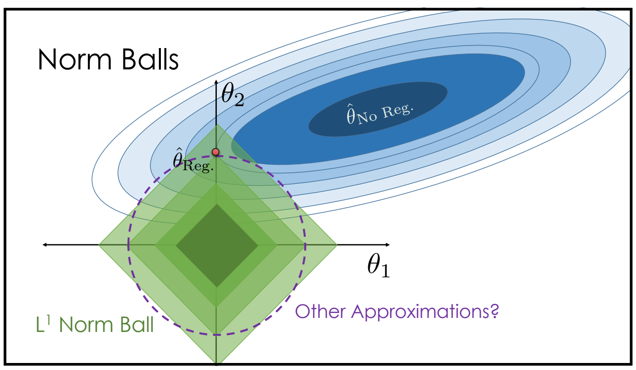


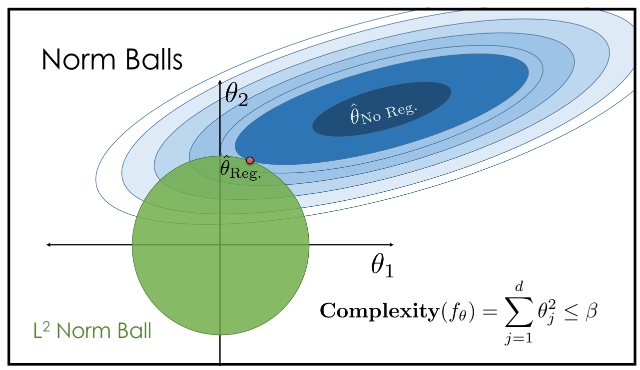
Convex approximation!

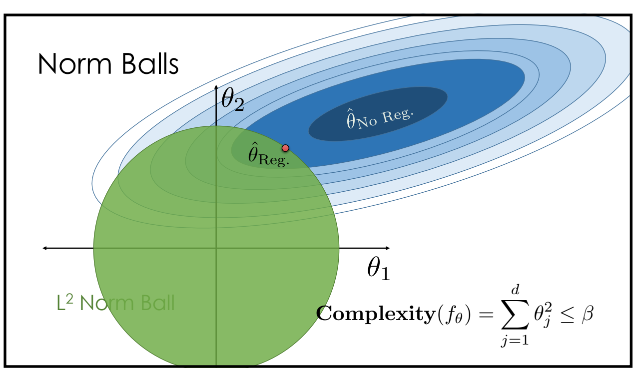
$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$$


Norm Balls
θ_2
$\hat{\theta}_{\text{No Reg.}}$
$\hat{\theta}_{\text{Reg.}}$
θ_1
Convex approximation!
L1 Norm Ball
$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$


Norm Balls
θ_2
$\hat{\theta}_{\text{No Reg.}}$
$\hat{\theta}_{\text{Reg.}}$
$\beta = 1$
$\beta = 2$
θ_1
Convex approximation!
L1 Norm Ball
$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} |\theta_j| \leq \beta$


Norm Balls
θ_2
$\hat{\theta}_{\text{No Reg.}}$
$\hat{\theta}_{\text{Reg.}}$
θ_1
L1 Norm Ball
Other Approximations?


Norm Balls
θ_2
$\hat{\theta}_{\text{No Reg.}}$
$\hat{\theta}_{\text{Reg.}}$
θ_1
L2 Norm Ball
$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \theta_j^2 \leq \beta$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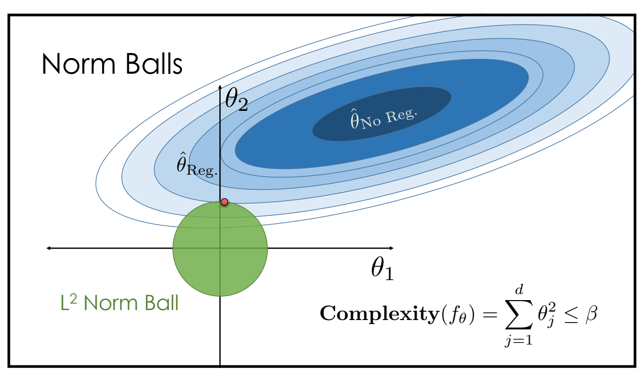
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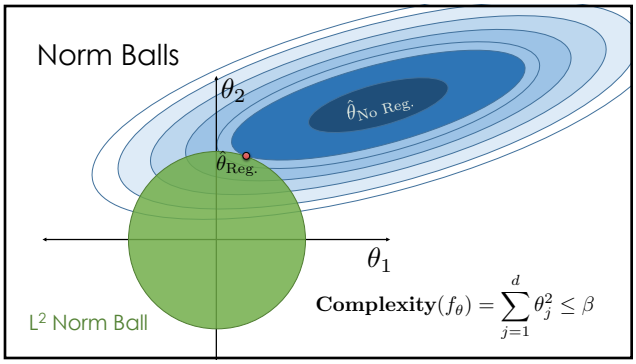
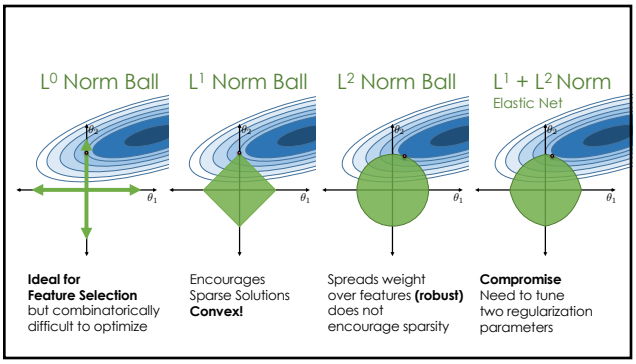




Generic Regularization (Constrained)

- Defining $\text{Complexity}(f_\theta) = R(\theta)$

$$\hat{\theta} = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \text{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that: $R(\theta) \leq \beta$

- There is an equivalent unconstrained formulation (obtained by Lagrangian duality)

Generic Regularization (Constrained)

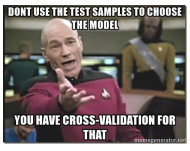
- Defining $\text{Complexity}(f_\theta) = R(\theta)$

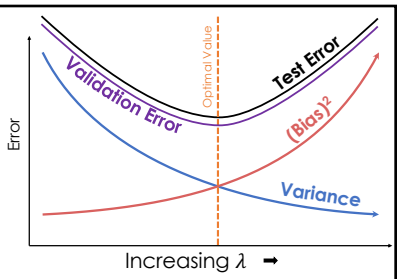
$$\hat{\theta} = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \text{Loss}\left(y_i, f_\theta(x_i)\right) + \lambda R(\theta)$$

Regularization Parameter

- There is an equivalent unconstrained formulation (obtained by Lagrangian duality)

Determining the Optimal λ





- Value of λ determines bias-variance tradeoff
  - Larger values → more regularization → more bias → less variance
- Determined through cross validation

Using Scikit-Learn for Regularized Regression

```
import sklearn.linear_model
```

- Regularization parameter α = 1/λ
  - larger α → less regularization → greater complexity → overfitting
- Lasso Regression (L1)
  - `linear_model.Lasso(alpha=3.0)`
  - `linear_model.LassoCV()` automatically picks α by cross-validation
- Ridge Regression (L2)
  - `linear_model.Ridge(alpha=3.0)`
  - `linear_model.RidgeCV()` automatically selects α by cross-validation
- Elastic Net (L1 + L2)
  - `linear_model.ElasticNet(alpha=3.0, l1_ratio = 2.0)`
  - `linear_model.ElasticNetCV()` automatically picks α by cross-validation

Standardization and the **Intercept** Term

Height = θ_1 age_in_seconds + θ_2 weight_in_tons

(θ_1: Small; θ_2: Large)

- Regularization penalized dimensions equally
- **Standardization**
  - Ensure that each dimensions has the same scale
  - centered around zero
- **Intercept Terms**
  - Typically don't regularize intercept term
  - Center y values (e.g., subtract mean)

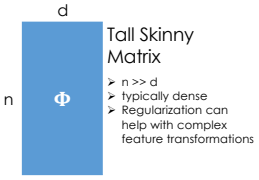
Standardization

For each dimension k:

$$z_k = \frac{x_k - \mu_k}{\sigma_k}$$

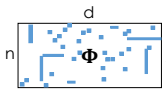
Regularization and **High-Dimensional Data**

Regularization is often used with high-dimensional data



Tall Skinny Matrix

- n >> d
- typically dense
- Regularization can help with complex feature transformations

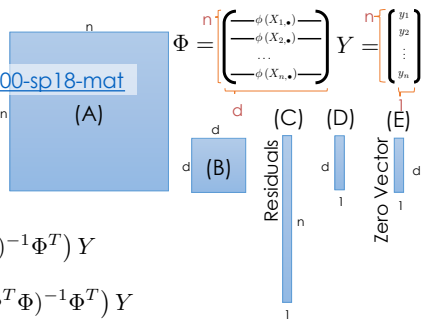


High-dimensional sparse matrix

- d > n
- **requires** regularization
- **Goal:** to determine **informative dimensions**
  - Consider L1 Regularization. Why?
- **Goal:** is to make **robust predictions**
  - Consider L2 (+L1) Regularization

Matching!

http://bit.ly/ds100-sp18-mat



1) $\Phi^T \Phi$

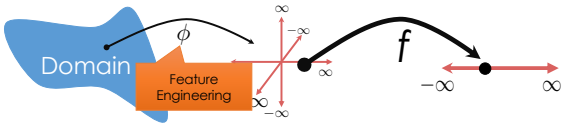
2) $\Phi^T Y$

3) $\left(I - \Phi(\Phi^T \Phi)^{-1} \Phi^T\right) Y$

4) $\Phi^T \left(I - \Phi(\Phi^T \Phi)^{-1} \Phi^T\right) Y$

Classification

Recap: *Least Squares Regression*

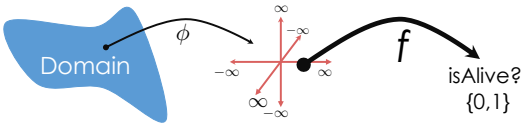


Squared Loss

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2 + \lambda \mathbf{R}(\theta)$$

Regularization

Classification

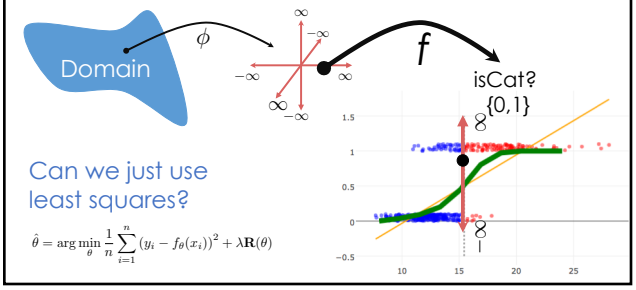


Can we just use least squares?

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2 + \lambda \mathbf{R}(\theta)$$

Python Demo

Classification



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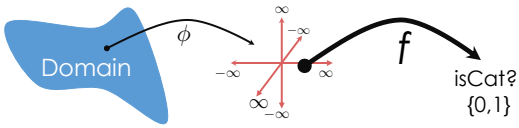
Classification



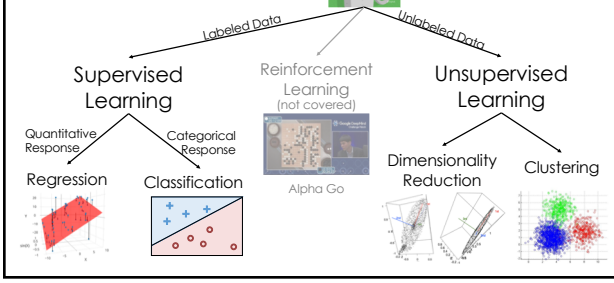
Can we just use least squares?

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2 + \lambda \mathbf{R}(\theta)$$

- Yes … (can be eg…
- Ne… (e…
- Difficult to interpret model …

Don't use Least Squares for **Classification**

Taxonomy of Machine Learning



Kinds of Classification

- **Binary** classification: Two classes
  - Examples: *Spam/Not Spam, churn/stay*
- **Multiclass** classification: Many classes (>2)
  - Examples: *Image labeling (Cat, Dog, Car), Next word in a sentence …*
- **Structured prediction** tasks (Classification)
  - Multiple related predictions
  - Examples: *Translation, Voice recognition*

Defining the Model

Logistic Regression

- Widely used models for **binary classification:**

$x =$ "Get a FREE sample ..."

$\phi(x) = [2.0, 0.0, \ldots, 1.0, 0.5]$ ➡ $y = 1$

1 = "Spam"
0 = "Ham"

Why is ham good and spam bad? ... (https://www.youtube.com/watch?v=anwy2MPT5RE)

- Models the probability of *y=1* given x

$$\hat{\mathbf{P}}_\theta(y = 1 \mid x) = \sigma(\phi(x)^T\theta) = \frac{1}{1 + \exp(-\phi(x)^T\theta)}$$

Logistic Regression

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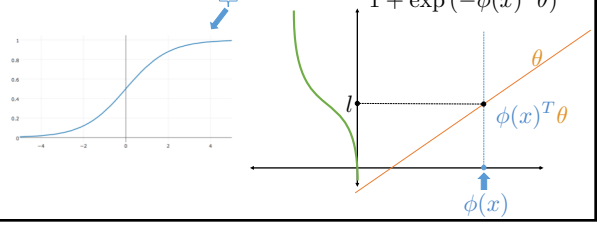
- Models the probability of *y=1* given x

$$\hat{\mathbf{P}}_\theta(y = 1 \mid x) = \sigma(\phi(x)^T\theta) = \frac{1}{1 + \exp(-\phi(x)^T\theta)}$$

$$\hat{\mathbf{P}}_\theta(y = 0 \mid x) = 1 - \hat{\mathbf{P}}_\theta(y = 1 \mid x)$$

Logistic Regression

Model: $\hat{\mathbf{P}}_\theta(y = 1 \mid x) = \sigma(\phi(x)^T\theta) = \frac{1}{1 + \exp(-\phi(x)^T\theta)}$



Python Demo

The Logistic Regression Model

Model: $\hat{\mathbf{P}}_\theta(y = 1 \mid x) = \sigma(\phi(x)^T\theta) = \frac{1}{1 + \exp(-\phi(x)^T\theta)}$

How do we fit the model to the data?

Defining the Loss

The Logistic Regression Model

Model: $\hat{\mathbf{P}}_\theta(y=1\,|\,x) = \sigma(\phi(x)^T\theta) = \dfrac{1}{1+\exp(-\phi(x)^T\theta)}$

The data:

$x =$ "Get a FREE sample ..." ➡ $y=1$

$\phi(x) = [2.0, 0.0, \ldots, 1.0, 0.5]$

Corresponding probability:

$\mathbf{P}(y=1\,|\,x) = 1 \qquad \mathbf{P}(y=0\,|\,x) = 0$

Loss Function

- We want our model to be close to the data:

$$\hat{\mathbf{P}}_\theta(y=1\,|\,x) \approx \mathbf{P}(y=1\,|\,x)$$

- Kullback–Leibler (KL) Divergence
  - For a **single** (x,y) data point

$$\mathbf{D}_{KL}(\mathbf{P}\,||\,\hat{\mathbf{P}}_\theta) = \sum_{k=1}^{K=2} \mathbf{P}(y=k\,|\,x)\log\left(\frac{\mathbf{P}(y=k\,|\,x)}{\hat{\mathbf{P}}_\theta(y=k\,|\,x)}\right)$$

Binary Classification

  - Average KL Divergence for all the data:

- Kullback–Leibler (KL) Divergence
  - For a **single** (x,y) data point

$$\mathbf{D}_{KL}(\mathbf{P}\,||\,\hat{\mathbf{P}}_\theta) = \sum_{k=1}^{K=2} \mathbf{P}(y=k\,|\,x)\log\left(\frac{\mathbf{P}(y=k\,|\,x)}{\hat{\mathbf{P}}_\theta(y=k\,|\,x)}\right)$$

Binary Classification

  - Average KL Divergence for all the data:

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K} \mathbf{P}(y_i=k\,|\,x_i)\log\left(\frac{\mathbf{P}(y_i=k\,|\,x_i)}{\hat{\mathbf{P}}_\theta(y_i=k\,|\,x_i)}\right)$$

Log(a/b) = Log(a) – Log(b)

Doesn't depend on θ

$$\cancel{\mathbf{P}(y_i=k\,|\,x_i)\log(\mathbf{P}(y_i=k\,|\,x_i))} - \mathbf{P}(y_i=k\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=k\,|\,x_i)\right)$$

- Average **cross entropy loss**

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K=2} -\mathbf{P}(y_i=k\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=k\,|\,x_i)\right)$$

Binary Classification

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n} -\mathbf{P}(y_i=1\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=1\,|\,x_i)\right) - \mathbf{P}(y_i=0\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=0\,|\,x_i)\right)$$

$\mathbf{P}(y_i=1\,|\,x_i) = y_i$	$\hat{\mathbf{P}}_\theta(y_i=1\,|\,x_i) = \sigma(\phi(x_i)^T\theta)$
$\mathbf{P}(y_i=0\,|\,x_i) = (1-y_i)$	$\hat{\mathbf{P}}_\theta(y_i=0\,|\,x_i) = 1-\sigma(\phi(x_i)^T\theta)$

- Average **cross entropy loss**

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K=2} -\mathbf{P}(y_i=k\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=k\,|\,x_i)\right)$$

Binary Classification

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n} -\quad y_i \quad \log\left(\quad \sigma(\phi(x_i)^T\theta)\quad\right) - \quad (1-y_i) \quad \log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

- Average **cross entropy loss**

$$\arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K=2} -\mathbf{P}(y_i=k\,|\,x_i)\log\left(\hat{\mathbf{P}}_\theta(y_i=k\,|\,x_i)\right)$$

Binary Classification

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i\log\left(\sigma(\phi(x_i)^T\theta)\right) + (1-y_i)\log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

Expanding

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i\log\left(\sigma(\phi(x_i)^T\theta)\right) + \log\left(1-\sigma(\phi(x_i)^T\theta)\right) - y_i\log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

Grouping Terms

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \log\left(\sigma(\phi(x_i)^T\theta)\right) + \log\left(1-\sigma(\phi(x_i)^T\theta)\right) - y_i \log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

Grouping Terms

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \log\left(\frac{\sigma(\phi(x_i)^T\theta)}{1-\sigma(\phi(x_i)^T\theta)}\right) + \log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

$$\log \frac{\frac{1}{1+\exp(-\phi(x_i)^T\theta)} \times \left(1+\exp\left(-\phi(x_i)^T\theta\right)\right)}{1-\frac{1}{1+\exp(-\phi(x_i)^T\theta)} \times \left(1+\exp\left(-\phi(x_i)^T\theta\right)\right)}$$

$$\overset{\text{Alg.}}{=} \log \frac{1}{1+\exp\left(-\phi(x_i)^T\theta\right)-1} \overset{\text{Alg.}}{=} \log \exp\left(\phi(x_i)^T\theta\right) \overset{\text{Alg.}}{=} \phi(x_i)^T\theta$$

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \log\left(\frac{\sigma(\phi(x_i)^T\theta)}{1-\sigma(\phi(x_i)^T\theta)}\right) + \log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(1-\sigma(\phi(x_i)^T\theta)\right)$$

$$1-\frac{1}{1+\exp\left(-\phi(x_i)^T\theta\right)} \overset{\text{Defn. of } \sigma}{=} \frac{\exp\left(-\phi(x_i)^T\theta\right)}{1+\exp\left(-\phi(x_i)^T\theta\right)} \overset{\text{Alg.}}{=} \frac{1}{1+\exp\left(\phi(x_i)^T\theta\right)}$$

$\times \exp\left(\phi(x_i)^T\theta\right)$

Definition

$\sigma(\phi(x)^T\theta) = \frac{1}{1+\exp\left(-\phi(x)^T\theta\right)}$

Defn. of σ

$$= \sigma\left(-\phi(x_i)^T\theta\right)$$

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

The Loss for Logistic Regression

- Average **cross entropy** (simplified):

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

- Equivalent to (derived from) **minimizing the KL divergence**
- Also equivalent to **maximizing the log-likelihood of the data** … (not covered in DS100 this semester)

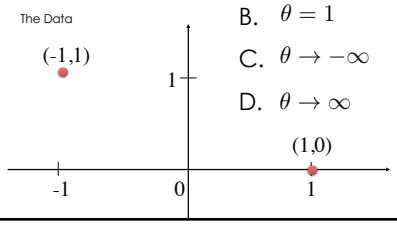
Is this loss function reasonable?

What is the value of θ?

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)\cdot\theta + \log(\sigma(-\phi(x_i)\cdot\theta))$$

Assume: $\phi(x) = x$

The Data

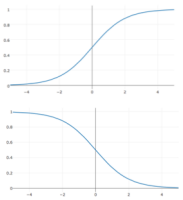


A. $\theta = -1$

B. $\theta = 1$

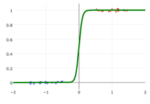
C. $\theta \to -\infty$

D. $\theta \to \infty$



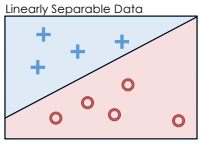
Linearly Separable Data

- A classification dataset is said to be linearly separable if there exists a hyperplane that separates the two classes.
- If data is linearly separable, logistic regression requires regularization

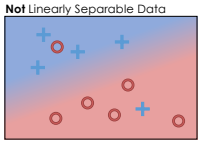


Weights go to infinity!

Linearly Separable Data



Not Linearly Separable Data



Logistic Loss Function

- Average KL divergence (simplified)

$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

- Take Derivative:

$$\nabla_\theta \mathbf{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \nabla_\theta y_i \phi(x_i)^T\theta + \nabla_\theta \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

$$= -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \nabla_\theta \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

- Average KL divergence (simplified)

$$\arg\min_{\theta} -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

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$$= -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \nabla_\theta \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$
$$= -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \frac{1}{\sigma\left(-\phi(x_i)^T\theta\right)}\nabla_\theta \sigma\left(-\phi(x_i)^T\theta\right)$$

- Take Derivative:

$$\nabla_\theta \mathbf{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \frac{1}{\sigma\left(-\phi(x_i)^T\theta\right)}\nabla_\theta \sigma\left(-\phi(x_i)^T\theta\right)$$

Useful Identity

$$\frac{\partial}{\partial t}\sigma(t) = \frac{\partial}{\partial t}\frac{1}{1+e^{-t}} \overset{\text{Chain Rule}}{=} \frac{-1}{(1+e^{-t})^2}\frac{\partial}{\partial t}\left(1+e^{-t}\right)$$
$$\overset{\text{Chain Rule}}{=} \frac{e^{-t}}{(1+e^{-t})^2} \overset{\text{Alg.}}{=} \left(\frac{1}{1+e^{-t}}\right)\left(\frac{e^{-t}}{1+e^{-t}}\right)$$
$$\overset{\text{Alg.}}{=} \left(\frac{1}{1+e^{-t}}\right)\left(\frac{1}{e^{t}+1}\right) \overset{\text{Defn. of } \sigma}{=} \sigma(t)\sigma(-t)$$

- Take Derivative:

$$\nabla_\theta \mathbf{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \frac{1}{\sigma\left(-\phi(x_i)^T\theta\right)}\nabla_\theta \sigma\left(-\phi(x_i)^T\theta\right)$$

Useful Identity $\quad \frac{\partial}{\partial t}\sigma(t) = \sigma(t)\sigma(-t)$

$$= -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i) + \frac{\sigma\left(-\phi(x_i)^T\theta\right)}{\sigma\left(-\phi(x_i)^T\theta\right)}\sigma\left(\phi(x_i)^T\theta\right)\nabla_\theta(-\phi(x_i)^T\theta)$$

$$= -\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sigma\left(\phi(x_i)^T\theta\right)\right)\phi(x_i)$$

Logistic Loss Function

- Average KL divergence (simplified)

$$\arg\min_{\theta} -\frac{1}{n}\sum_{i=1}^{n} y_i \phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)$$

- Take Derivative:

$$\nabla_\theta \mathbf{L}(\theta) = -\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sigma\left(\phi(x_i)^T\theta\right)\right)\phi(x_i)$$

- Set derivative = 0 and solve for Θ
  - No general analytic solution
  - Solved using numeric methods

The Gradient Descent Algorithm

$\theta^{(0)} \leftarrow$ initial vector (random, zeros …)

For τ from 0 to convergence:

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \rho(\tau)\left(\nabla_\theta \mathbf{L}(\theta)\Big|_{\theta=\theta^{(\tau)}}\right) \quad \text{Evaluated at } \theta=\theta^{(\tau)}$$

- $\rho(\tau)$ is the step size (learning rate)
  - typically $1/\tau$
- Converges when gradient is ≈ 0 (or we run out of patience)

Gradient Descent for Logistic Regression

Logistic Regression

$\theta^{(0)} \leftarrow$ initial vector (random, zeros …)

For τ from 0 to convergence:

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \rho(\tau)\left(\frac{1}{n}\sum_{i=1}^{n}\left(\sigma\left(\phi(x_i)^T\theta^{(\tau)}\right) - y_i\right)\phi(x_i)\right)$$

- $\rho(\tau)$ is the step size (learning rate)
  - typically $1/\tau$
- Converges when gradient is ≈ 0 (or we run out of patience)

Demo!

Stochastic Gradient Descent

- For many learning problems the gradient is a sum:

$$\nabla_\theta \mathbf{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(\sigma\left(\phi(x_i)^T\theta\right) - y_i\right)\phi(x_i)$$

  - For large n this can be costly
- What if we approximated the gradient by looking at a few random points:

$$\nabla_\theta \mathbf{L}(\theta) \approx \frac{1}{|\mathcal{B}|}\sum_{i\in\mathcal{B}}\left(\sigma\left(\phi(x_i)^T\theta\right) - y_i\right)\phi(x_i)$$

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Batch Size

Random sample of records

- This is a reasonable estimator for the gradient
  - Unbiased …
- Often batch size is one! (why is this helpful)
  - Fast to compute!
- A key ingredient in the recent success of deep learning

Stochastic Gradient Descent

$\theta^{(0)} \leftarrow$ initial vector (random, zeros …)

For τ from 0 to convergence:

$\mathcal{B} \sim$ Random subset of indices

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \rho(\tau)\left(\frac{1}{|\mathcal{B}|}\sum_{i\in\mathcal{B}}\nabla_\theta \mathbf{L}_i(\theta)\Big|_{\theta=\theta^{(\tau)}}\right)$$

Decomposable Loss $\mathbf{L}(\theta) = \sum_{i=1}^{n}\mathbf{L}_i(\theta) = \sum_{i=1}^{n}\mathbf{L}(\theta, x_i, y_i)$

Loss can be written as a sum of the loss on each record.

Gradient Descent

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For τ from 0 to convergence:

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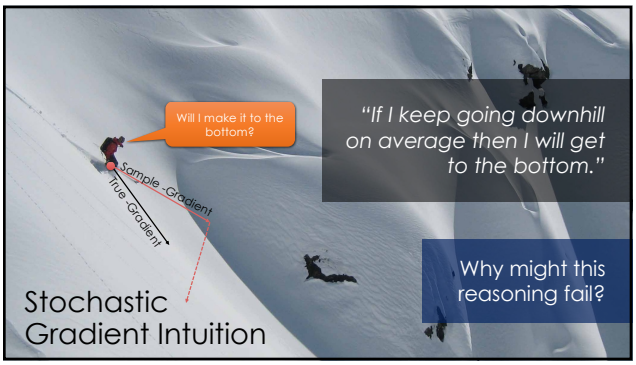
Very Similar Algorithms

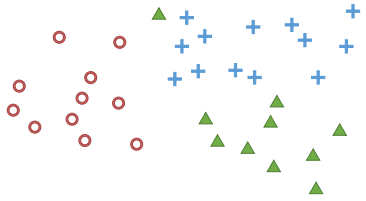
Assuming Decomposable Loss Functions



Python Demo!

Multiclass (more than 2) Classification

- **One-vs-rest** train separate binary classifiers for each class



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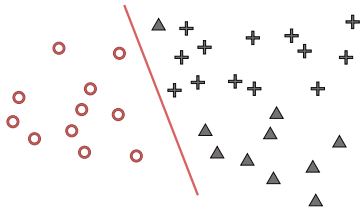

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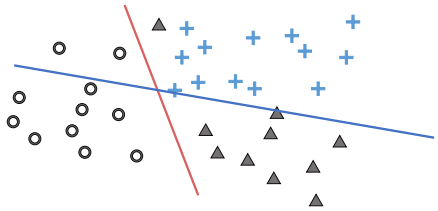

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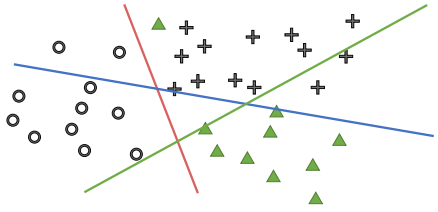

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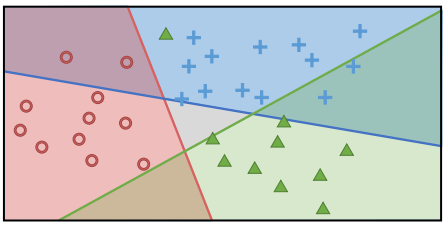
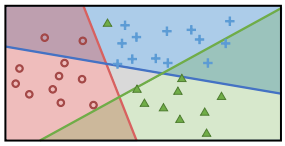


Multiclass (more than 2) Classification

- **One-vs-rest** train separate binary classifiers for each class
  - Class with highest confidence wins
  - Need to address class imbalance issue



- **Soft-Max** multiclass classification

- **Soft-Max** multiclass classification

$$\mathbf{P}(Y = j \mid x) = \frac{\exp\left(x^T \theta^{(j)}\right)}{\sum_{m=1}^{k} \exp\left(x^T \theta^{(m)}\right)}$$

- Separate $\theta^{(j)} \in \mathbb{R}^p$ for each class
- Trained using gradient descent methods
- Over parameterized. Why?
  - k sets of parameters one for each class
  - Only need k-1 parameters

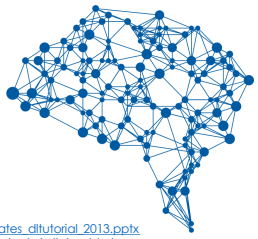
$$\mathbf{P}(y = k \mid x) = 1 - \sum_{j=1}^{K} \mathbf{P}(y = j \mid x)$$

- Often use k parameters + regularization to address lack of identifiability.

Python Demo!

Deep Learning Overview

Bonus Material

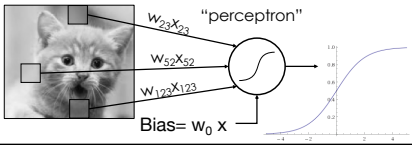


Borrowed heavily from excellent talks by:
- **Adam Coates:** http://ai.stanford.edu/~acoates/coates_dltutorial_2013.pptx
- **Fei-Fei Li and Andrej Karpathy:** http://cs231n.stanford.edu/syllabus.html

Logistic Regression as a "Neuron"

- Consider the simple function family: $\sigma(u) = \frac{1}{1+\exp(-u)}$

$$f_w(x) = \sigma\left(w^T x\right) = \sigma\left(\sum_{j=1}^{d} w_j x_j\right) = P(y = 1 \mid x)$$

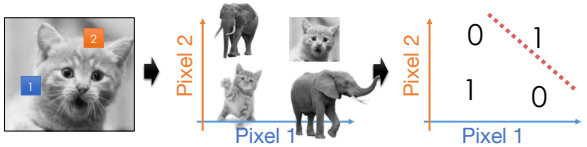


Neuron "fires" if weighted sum of input is greater than zero.

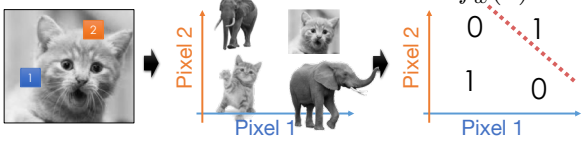
Logistic Regression: Strengths and Limitations

- Widely used machine learning technique
  - convex → efficient to learn
  - easy to interpret model weights
  - works well given good features

- Limitations:
  - Restricted to linear relationships → sensitive to choice of features

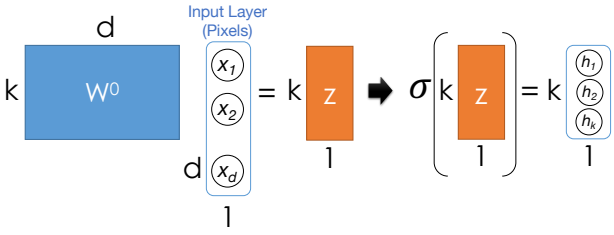


Feature Engineering

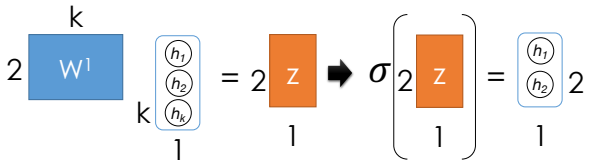


- Rather than use raw **pixels build/train feature functions**:

Composition Linear Models and Nonlinearities



Composition Linear Models and Nonlinearities

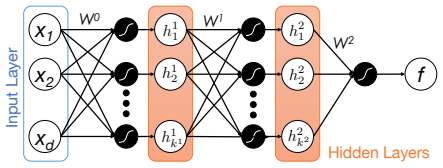


Neural Networks

- Composing "perceptrons"

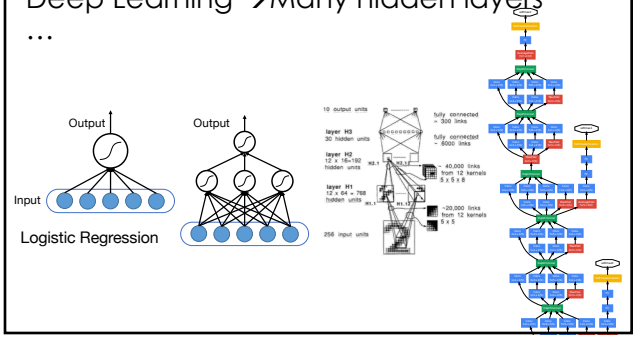
$$x \to \sigma(W^0 x) \to h^1 \to \sigma(W^1 h^1) \to h^2 \to \sigma(W^2 h^2) \to f$$

$$y = f_{W^0,W^1,W^2}(x) = \sigma\left(W^2\ \sigma\left(W^1\ \sigma\left(W^0 x\right)\right)\right)$$

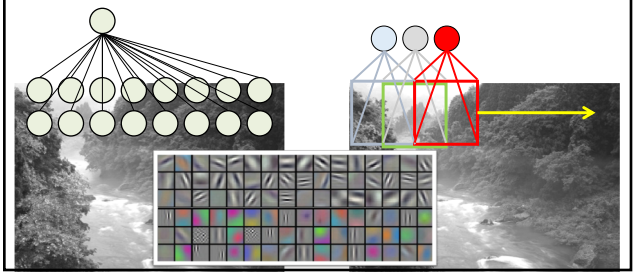


Deep Learning →Many hidden layers

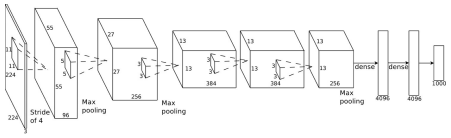
…



Convolutional Neural Networks: Exploiting Spatial Sparsity

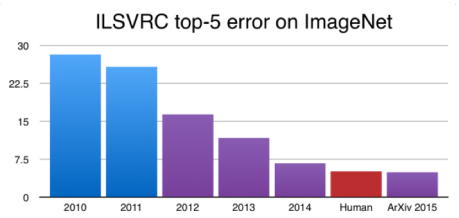


Example: AlexNet (Krizhevsky et al., NIPS 2012)

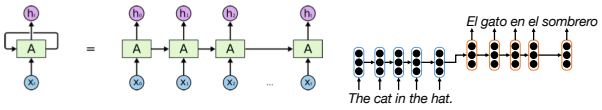


- Introduced in 2012, significantly outperformed state-of-the-art (top 5 error of 16% compared to runner-up with 26% error)
  - Covered in reading …

Improvement on ImagNet Benchmark

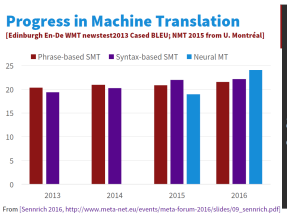


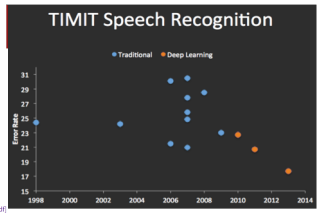
Recurrent Neural Networks: Modeling Sequence Structure



- State of the art in speech recognition and machine translation
  - Required LSTM and GRU to address long dependencies
- Similar to the HMM from classical Bayesian ML

Improvements in Machine Translation & Automatic Speech Recognition





Interested in Deep Learning?

- RISE Lab Deep Learning Overview:
  - https://ucbrise.github.io/cs294-rise-fa16/deep_learning.html
- TensorFlow Python Tutorial
- Stanford CS231 Labs
  - http://cs231n.github.io/linear-classify/
  - http://cs231n.github.io/optimization-1/
  - http://cs231n.github.io/optimization-2/