Classification & Logistic Regression

& maybe deep learning

Slides by:

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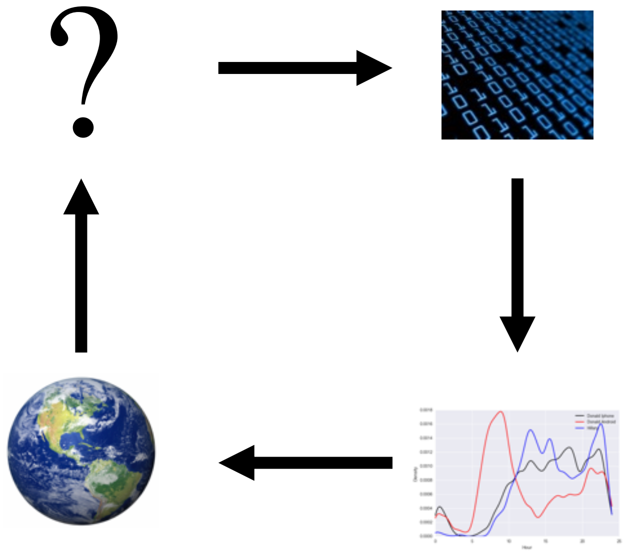
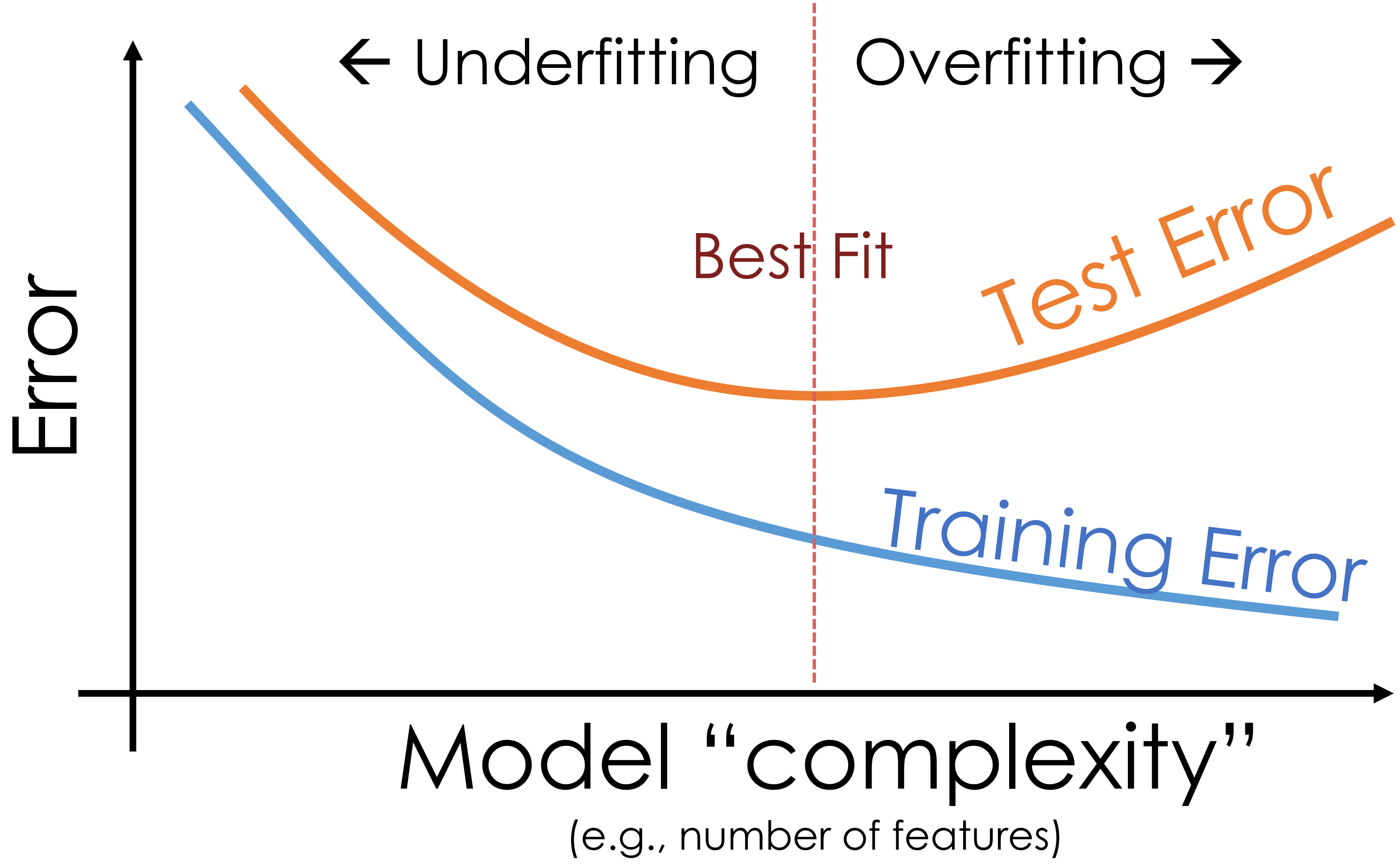


Previously…

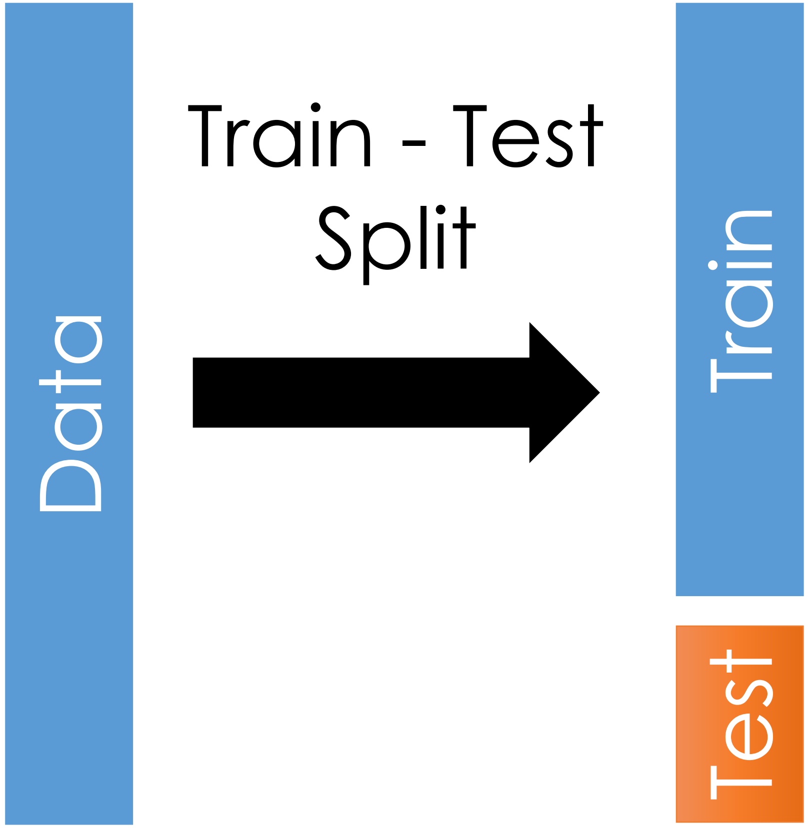
Training vs **Test** Error

Training error typically <u>*under estimates*</u> **test error**.



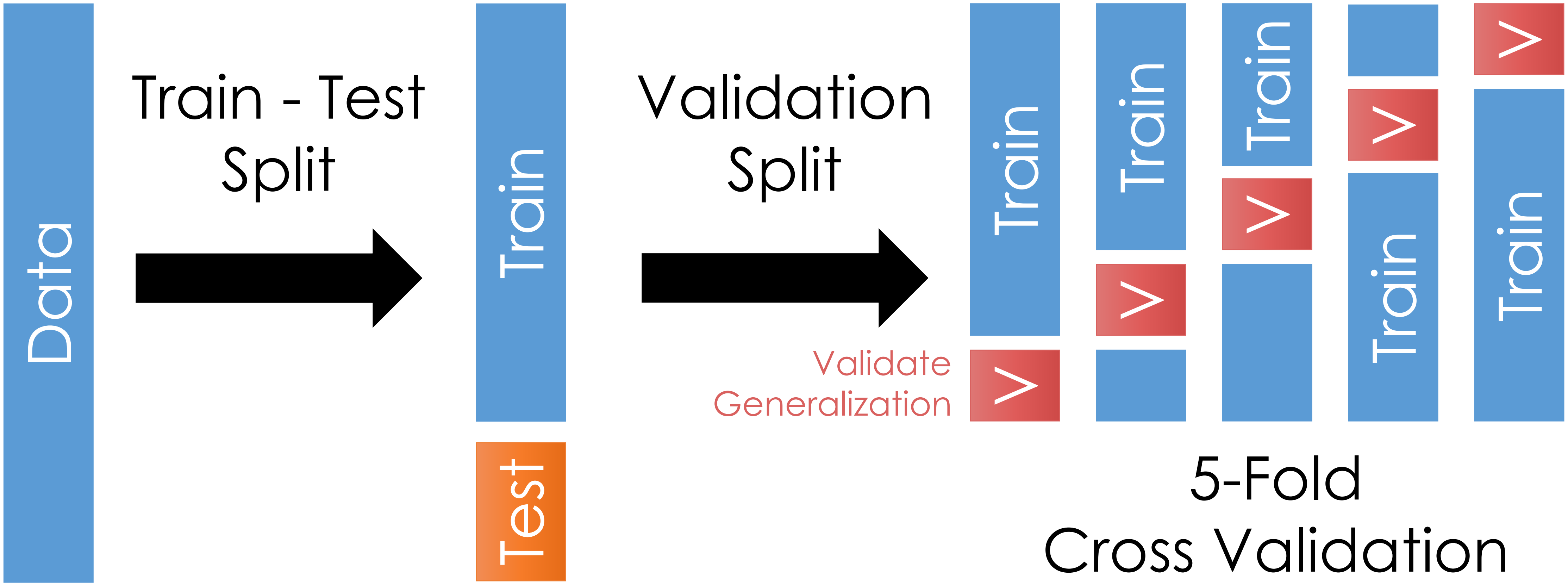
Generalization: *The Train-Test Split*

- **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*



Train - Test
Split

Validation
Split

Validate
Generalization

5-Fold
Cross Validation

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

Regularized Loss Minimization

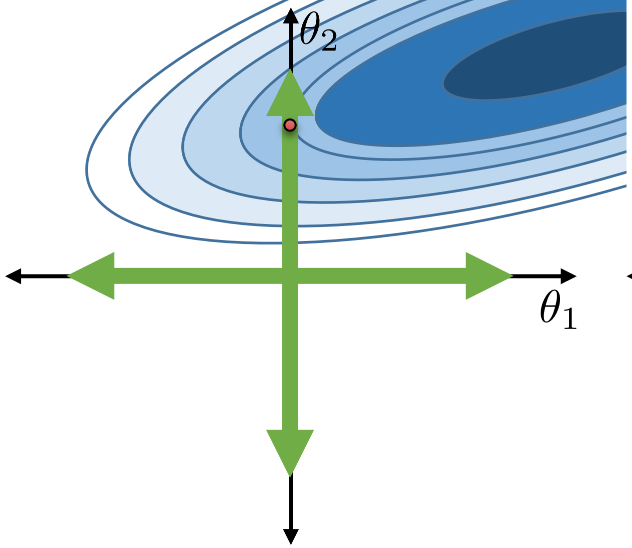
$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \textbf{Loss}\left(y_i, f_\theta(x_i)\right) \; + \lambda R(\theta)$$

Regularization Parameter

- Larger values of λ → more regularization
- **<u>Confusing!</u>:** Scikit-learn uses ***α* = 1/λ**
  - **Larger values of *α*** → <u>less regularization</u>

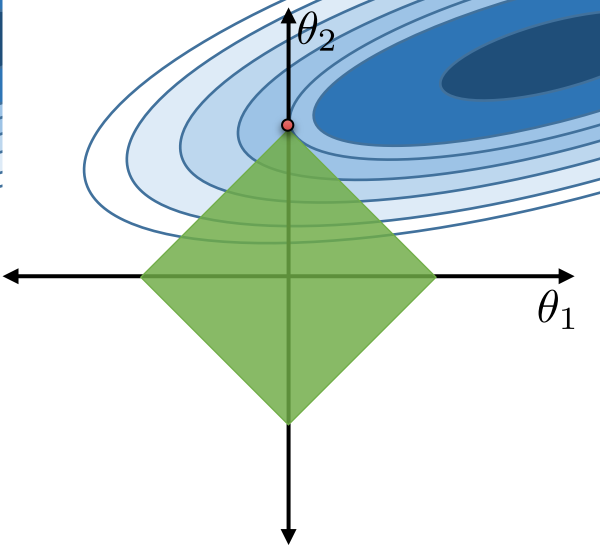
Different choices of $R(\theta)$

L^0 Norm Ball



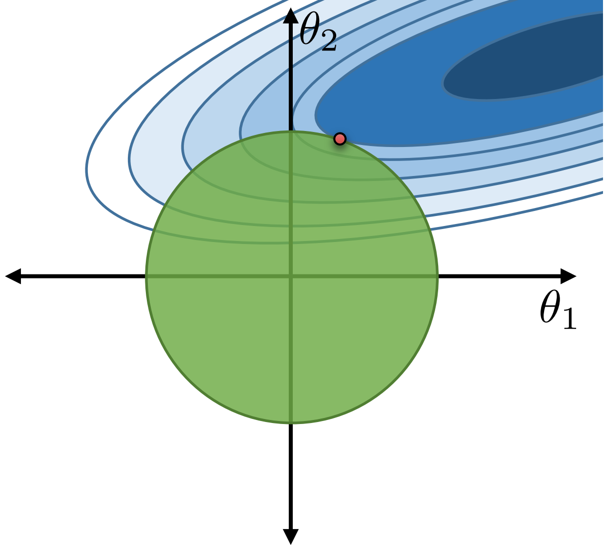
Ideal for
Feature Selection
but combinatorically
difficult to optimize

L^1 Norm Ball



Encourages
Sparse Solutions
Convex!

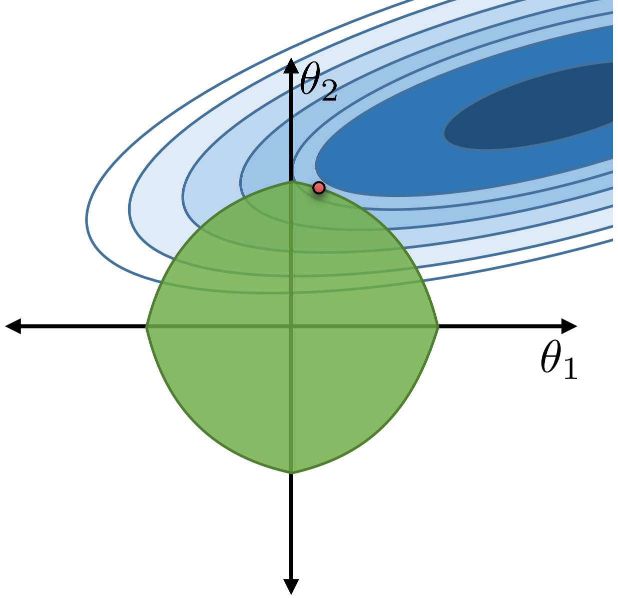
L^2 Norm Ball



Spreads weight
over features **(robust)**
does not
encourage sparsity

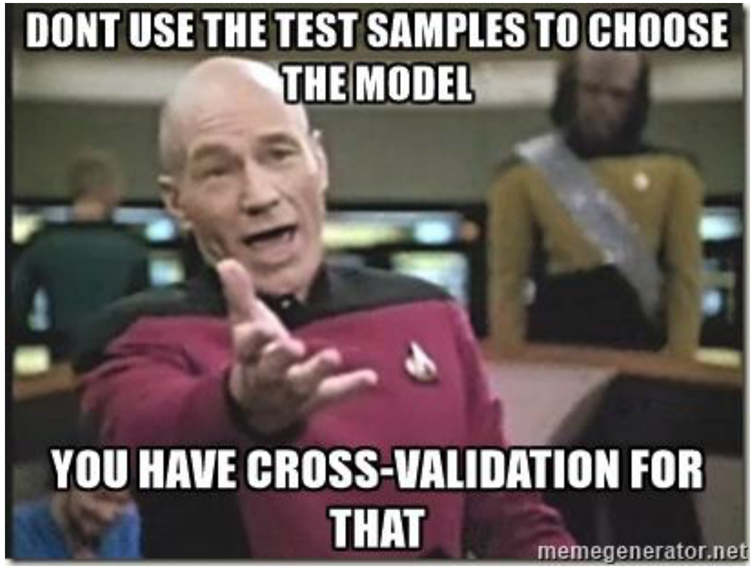
$L^1 + L^2$ Norm

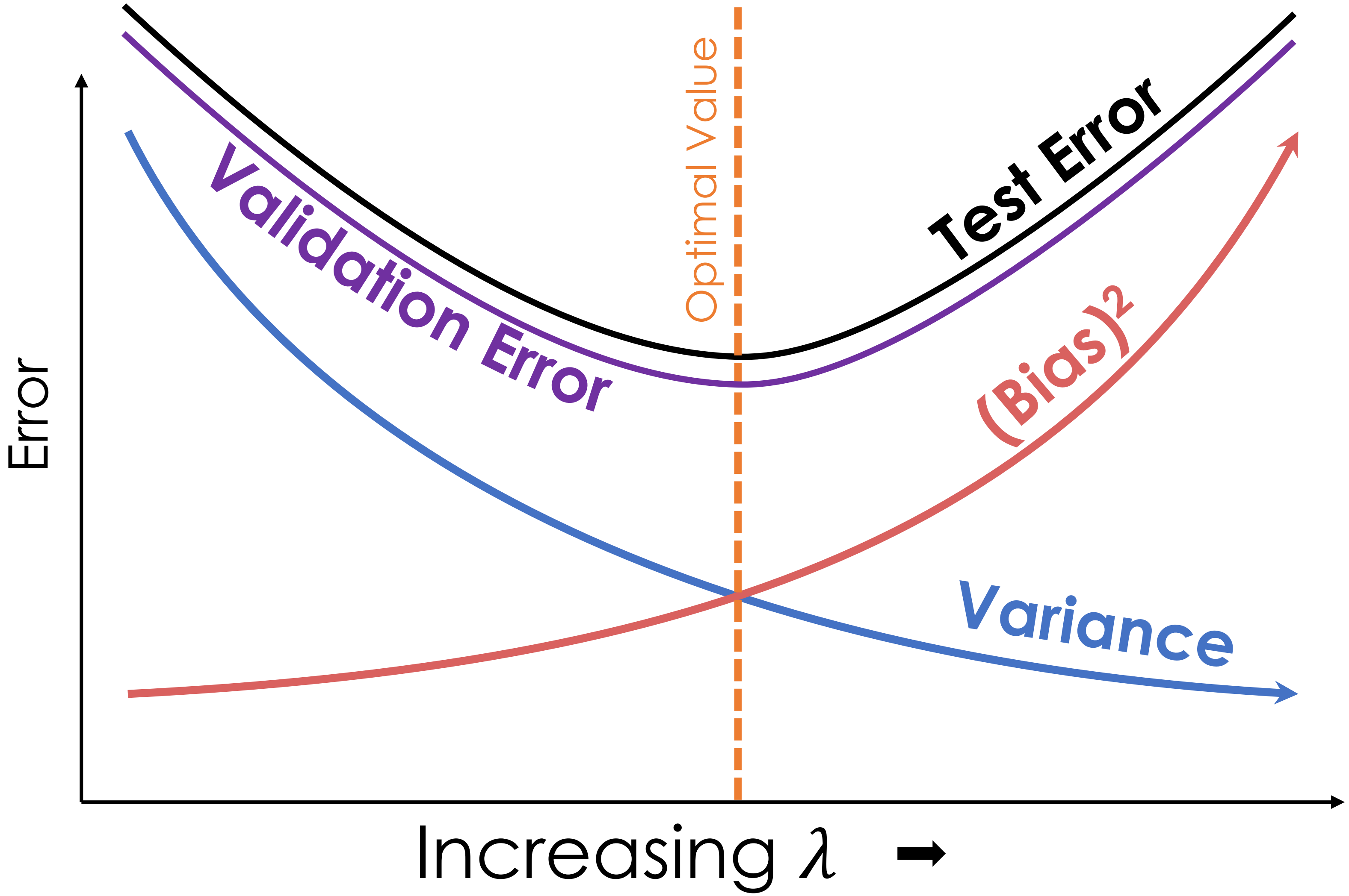
Elastic Net



Compromise
Need to tune
two regularization
parameters

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`

- <u>**Confusion Warning:**</u> 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

$$\texttt{Height} = \underbrace{\theta_1}_{\text{Small}} \texttt{age\_in\_seconds} + \underbrace{\theta_2}_{\text{Large}} \texttt{weight\_in\_tons}$$

- 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*:

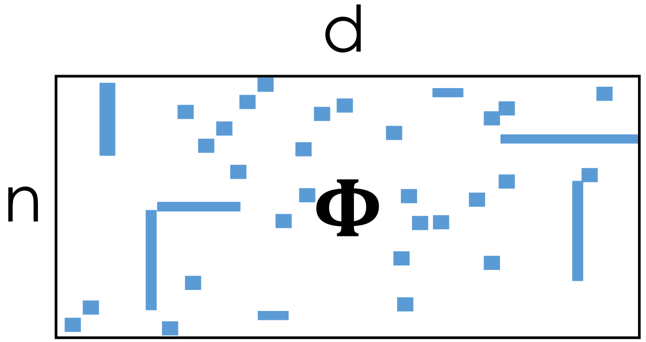
$$z_k = \frac{x_k - \mu_k}{\sigma_k}$$

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



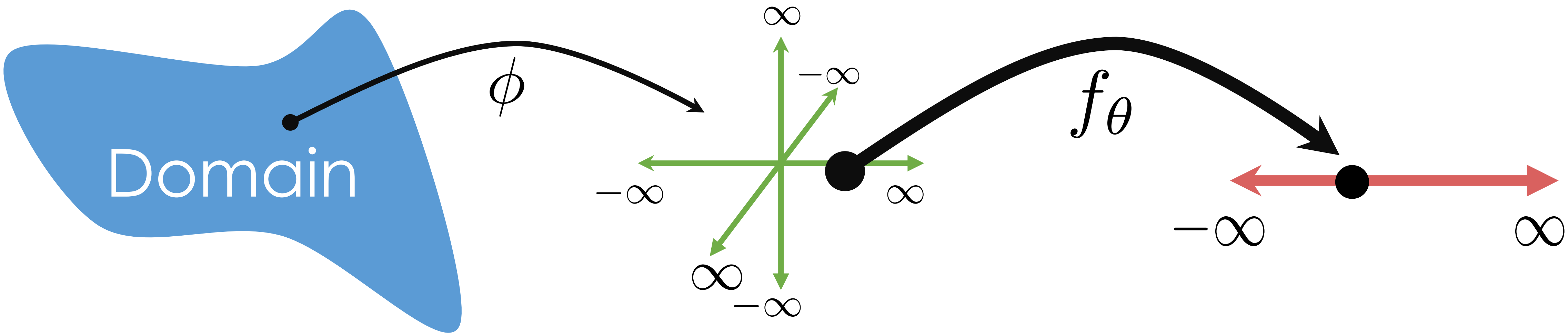
High-dimensional sparse matrix

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

Today

Classification

So far ....

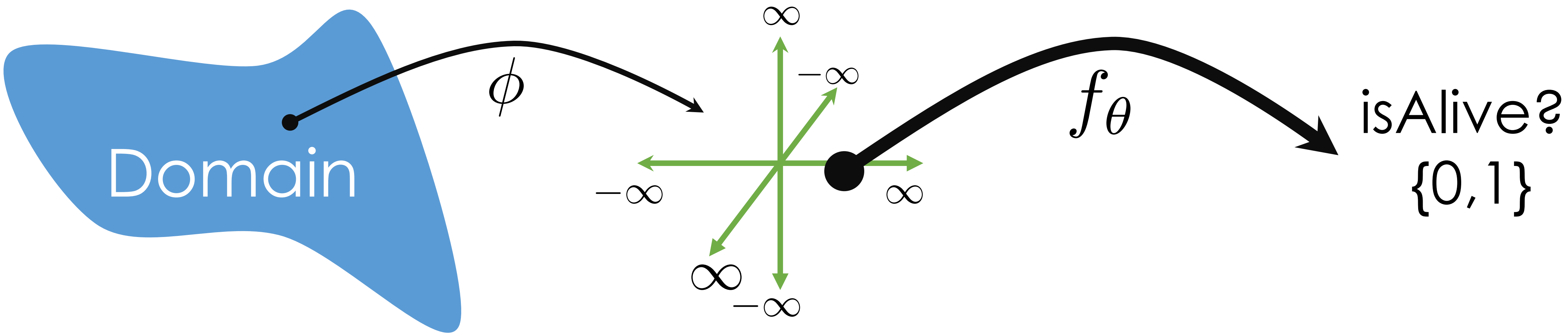


Squared Loss

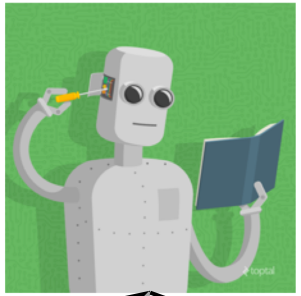
$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2 + \lambda \mathbf{R}(\theta)$$

Regularization

Classification



Taxonomy of Machine Learning



Labeled Data

Reward

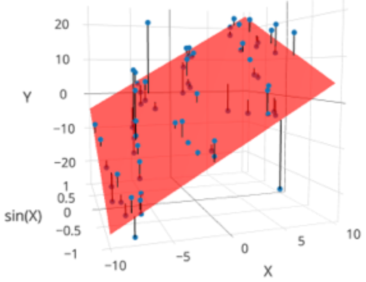
Unlabeled Data

Supervised Learning

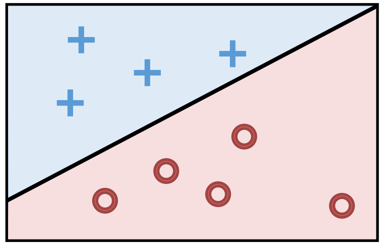
Quantitative Response

Categorical Response

Regression

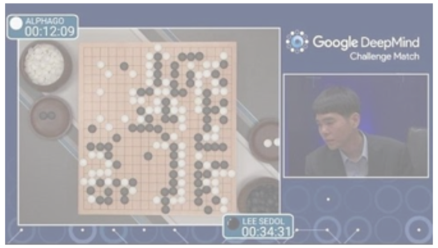


Classification



Reinforcement Learning

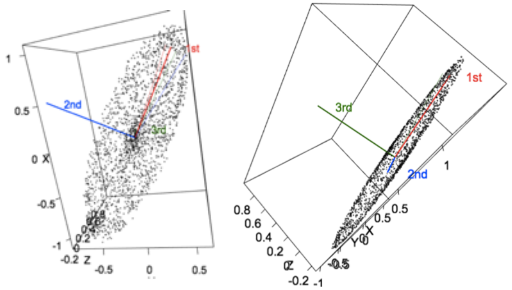
(not covered)



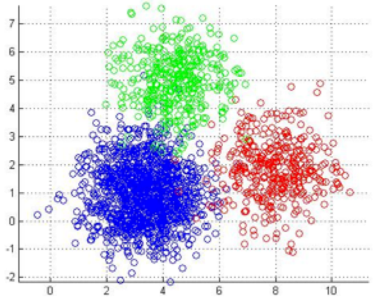
Alpha Go

Unsupervised Learning

Dimensionality Reduction



Clustering

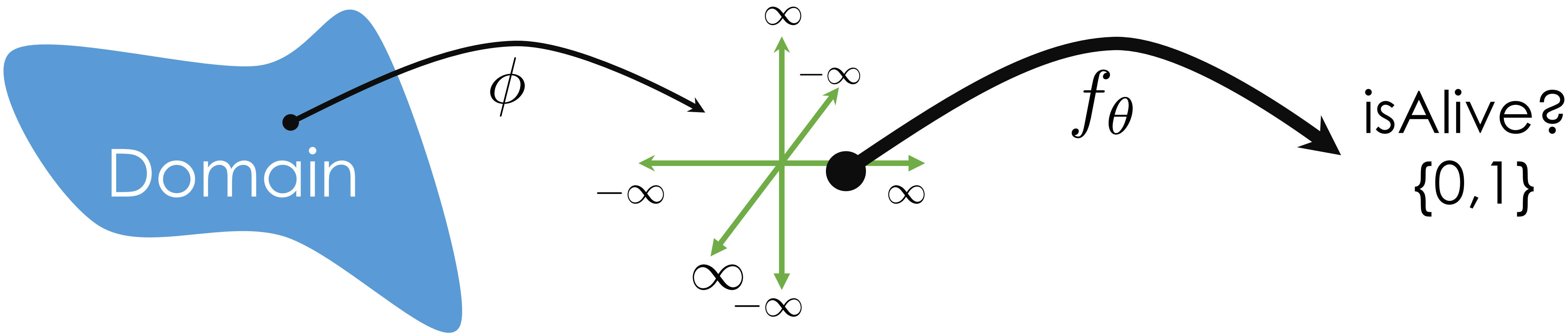


Kinds of Classification

Predicting a categorical variable

- **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*

Classification



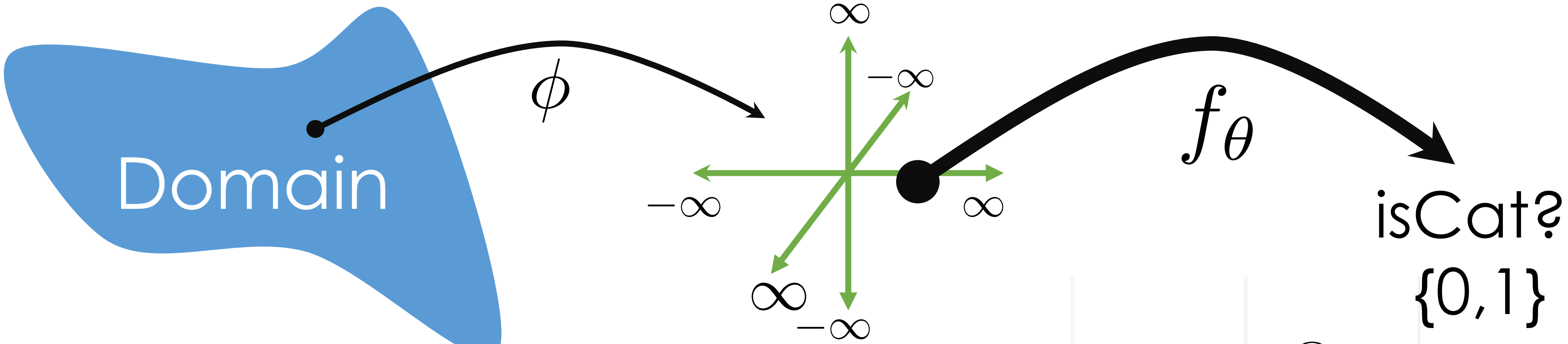
Can we just use least squares?

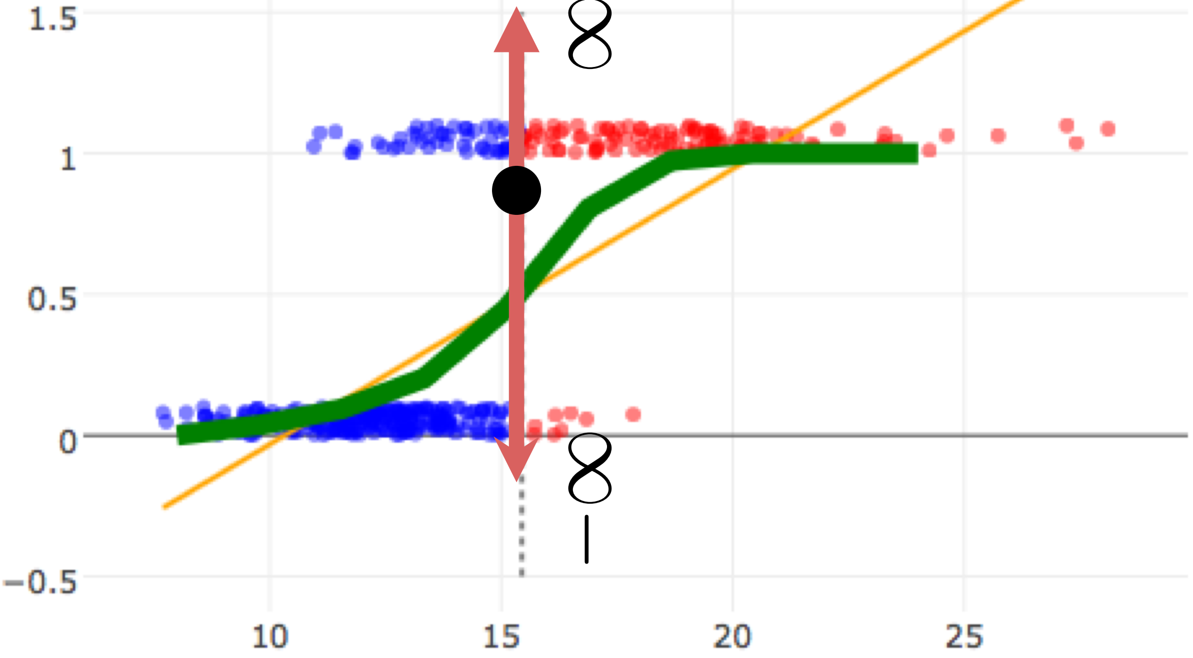
$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f_\theta(x_i)\right)^2 + \lambda \mathbf{R}(\theta)$$

Squared Loss

Python Demo

Classification





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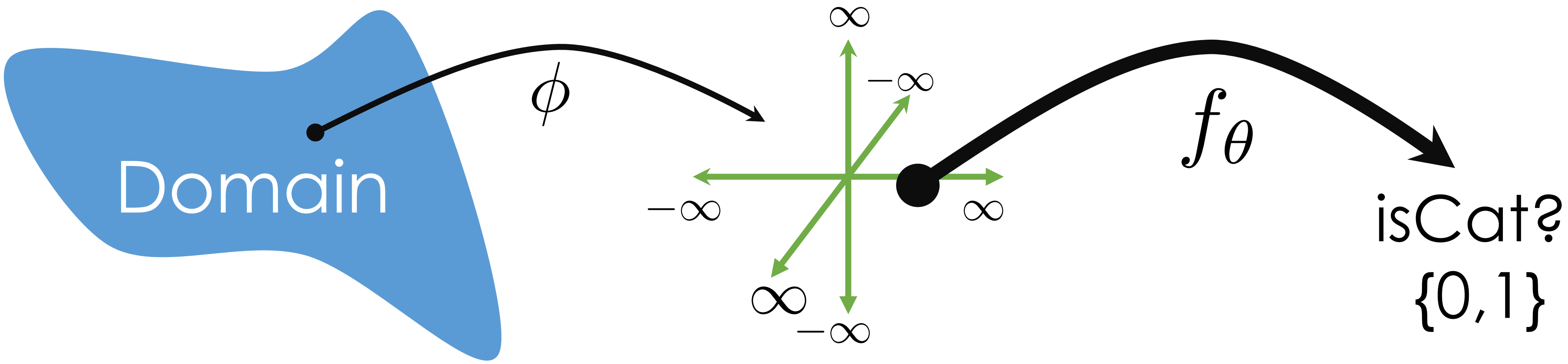


Can we just use least squares?

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

- ➢Yes …
- ➢Need
- ➢interpret model …
- ➢Sensitive to outliers

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

Defining a New Model for Classification

Logistic Regression

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

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

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

1 = "Spam"
0 = "Ham"

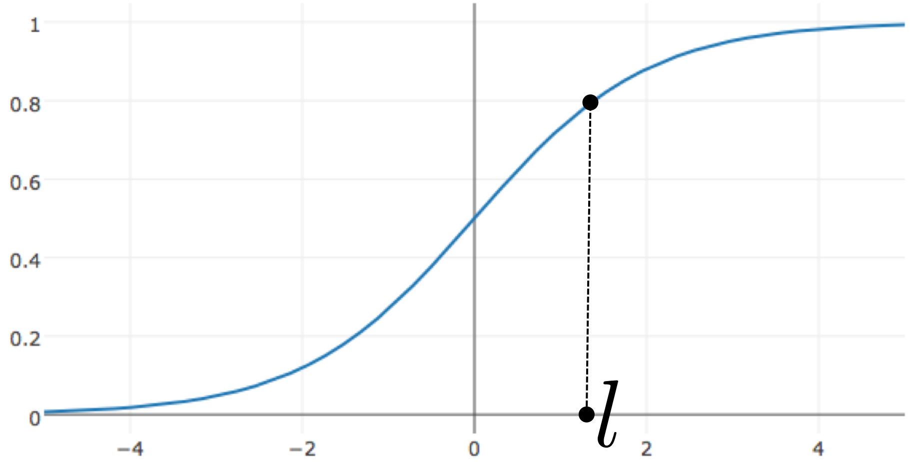
Why is ham good and spam bad? ... (https://www.youtube.com/watch?v=anwy2MPT5RE)

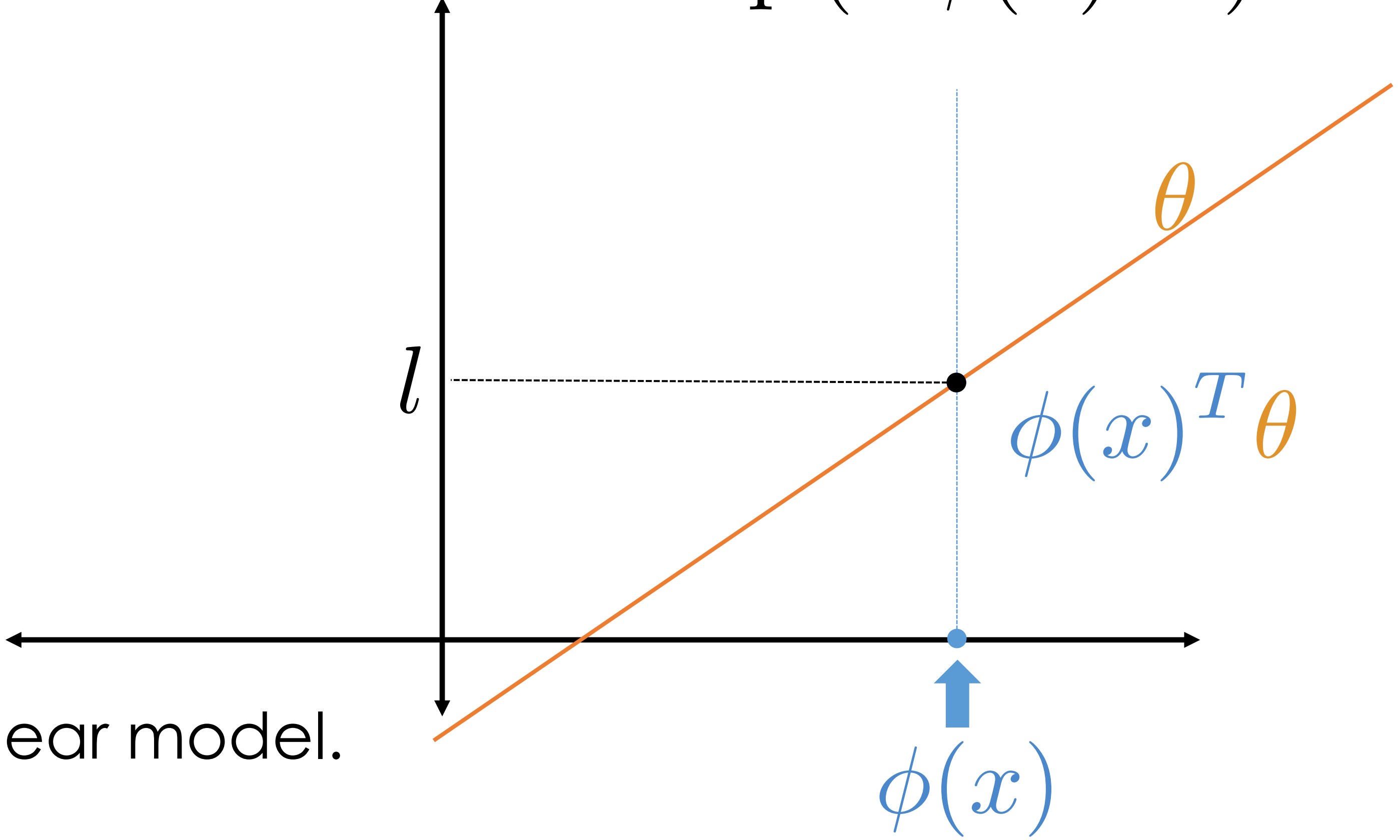
- Models the probability of *y=1* given x

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

Logistic Regression

Model: $$\hat{\mathbf{P}}_\theta\left(y = 1 \,|\, x\right) = \underbrace{\sigma}_{}\Big(\overbrace{\phi(x)^T\theta}^{\textbf{Linear Model}}\Big) = \frac{1}{1 + \exp\left(-\phi(x)^T\theta\right)}$$





Generalized Linear Model:
Non-linear transformation of a linear model.

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

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

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

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$$\hat{\mathbf{P}}_\theta\left(y = 0 \,|\, x\right) = 1 - \hat{\mathbf{P}}_\theta\left(y = 1 \,|\, x\right)$$

Python Demo

The Logistic Regression Model

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

How do we fit the model to the data?

Defining the Loss

Could we use the Squared Loss

- What about squared loss and the new model:

$$L(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sigma\left(\phi(x_i)^T \theta\right)\right)^2$$

  - Tries to match probability with 0/1 labels.
  - Occasionally used in some neural network applications
  - **Non-convex!**

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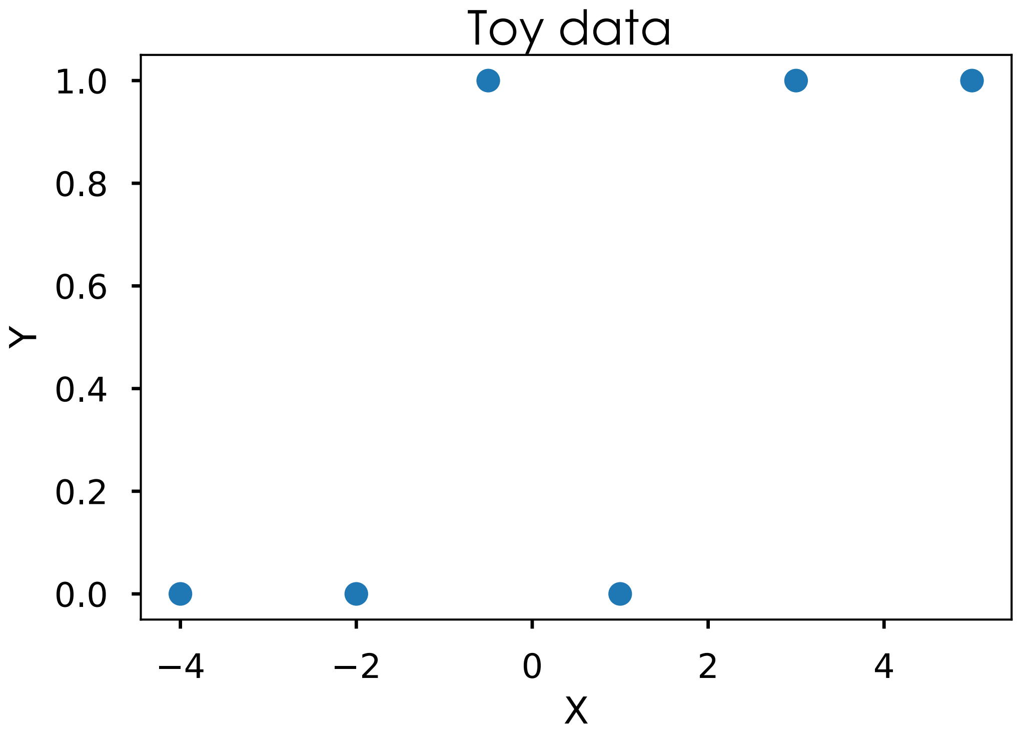
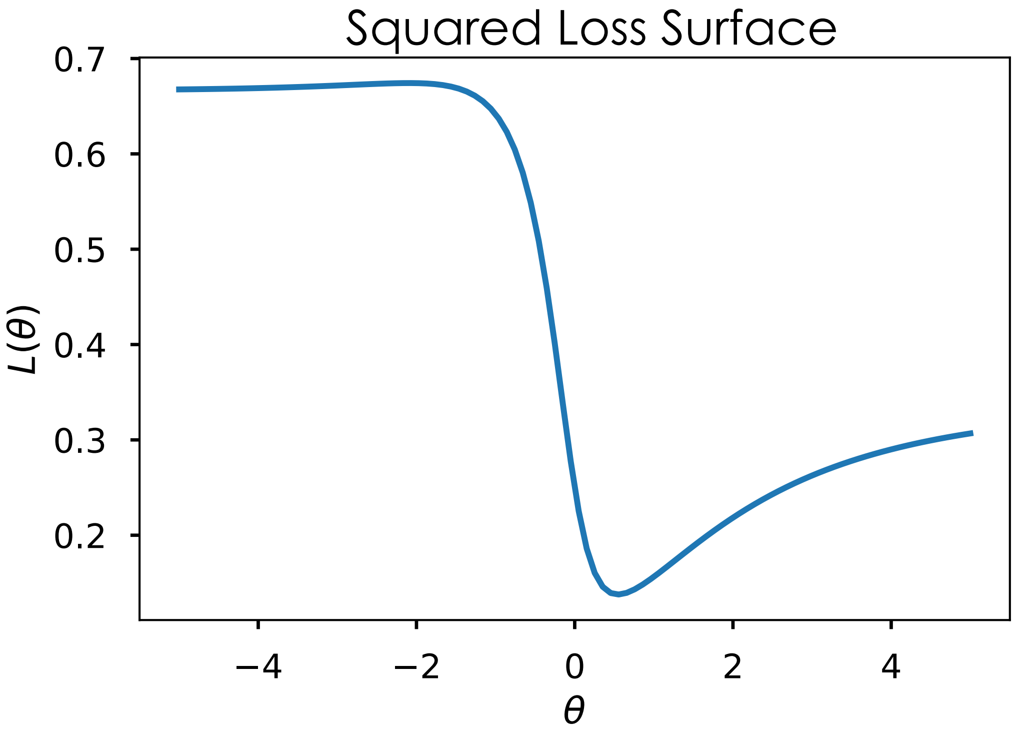




Defining the Cross Entropy Loss

Loss Function

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

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

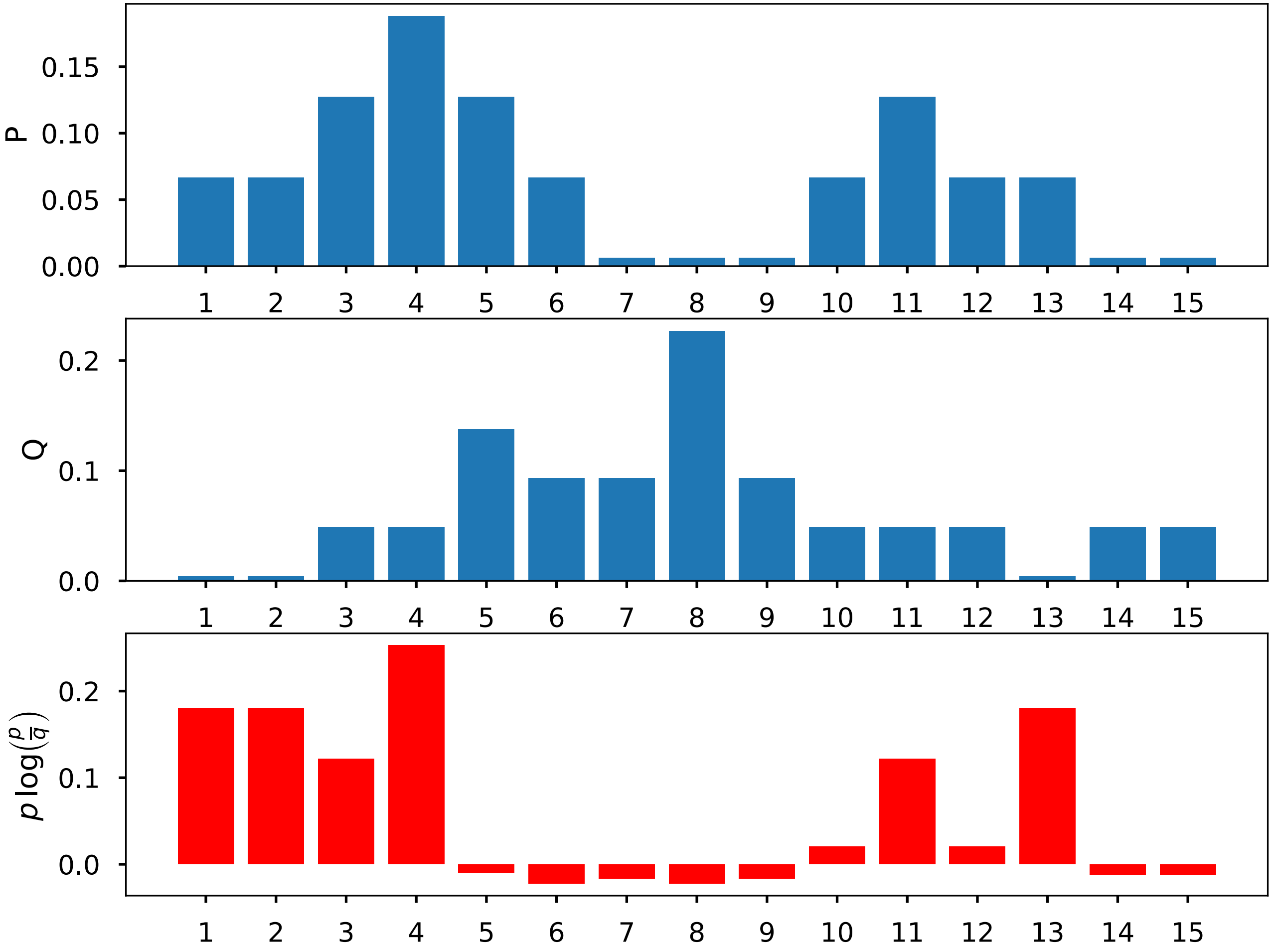
- Kullback–Leibler (KL) Divergence provides a measure of similarity between two distributions:
    - Between two discrete distributions P and Q

$$\mathbf{D}(P||Q)=\sum_{k=1}^{K}P(k)\log\left(\frac{P(k)}{Q(k)}\right)$$

Kullback–Leibler (KL) Divergence

$$\mathbf{D}(P||Q) = \sum_{k=1}^{K} P(k) \log\left(\frac{P(k)}{Q(k)}\right)$$

- ➢ The average log difference between P and Q weighted by P
- ➢ Does not penalize mismatch for rare events with respect to P



Loss Function

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

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

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

Binary Classification

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

  - Average KL Divergence for all the data:

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

Binary Classification

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

  - Average KL Divergence for all the data:

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

Doesn't depend on θ

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

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

- Average **cross entropy loss**

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

Summing from k = 0 to 1 and not k = 1 to 2 (to be consistent with 0/1 labels):

$$\arg\min_{\theta} -\frac{1}{n} \sum_{i=1}^{n} \left(\begin{array}{r} \mathbf{P}\left(y_i = 0 \mid x_i\right) \log\left(\hat{\mathbf{P}}_{\theta}\left(y_i = 0 \mid x_i\right)\right) + \\ \mathbf{P}\left(y_i = 1 \mid x_i\right) \log\left(\hat{\mathbf{P}}_{\theta}\left(y_i = 1 \mid x_i\right)\right) \end{array} \right)$$

$$\mathbf{P}\left(y_i = 1 \mid x_i\right) = y_i$$

$$\mathbf{P}\left(y_i = 0 \mid x_i\right) = \left(1 - y_i\right)$$

$$\hat{\mathbf{P}}_{\theta}\left(y_i = 1 \mid x_i\right) = \sigma(\phi(x_i)^T \theta)$$

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

- Average **cross entropy loss**

Binary Classification

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

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

Rewriting on one line:

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

- Average **cross entropy loss**

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

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

Expanding

$$\log\left(1 - \sigma\left(\phi(x_i)^T \theta\right)\right) - y_i \log\left(1 - \sigma\left(\phi(x_i)^T \theta\right)\right)$$

Grouping Terms

Copy & Paste

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

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

Definition

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

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

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

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

$$= \phi(x_i)^T\theta$$

Definition

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

A Linear mode of the “Log odds”

$$\log\left(\frac{\sigma\left(\phi(x_i)^T\theta\right)}{1-\sigma\left(\phi(x_i)^T\theta\right)}\right) = \underbrace{\phi(x_i)^T\theta}_{\text{Linear Model}} = \underbrace{\log\left(\frac{\hat{\mathbf{P}}_\theta\left(y_i = 1 \,|\, x_i\right)}{\hat{\mathbf{P}}_\theta\left(y_i = 0 \,|\, x_i\right)}\right)}_{\text{Log odds}}$$

A Linear mode of the "Log odds"

$$\log\left(\frac{\sigma\left(\phi(x_i)^T\theta\right)}{1-\sigma\left(\phi(x_i)^T\theta\right)}\right) = \underbrace{\phi(x_i)^T\theta}_{\text{Linear Model}} = \underbrace{\log\left(\frac{\hat{\mathbf{P}}_\theta\left(y_i = 1 \mid x_i\right)}{\hat{\mathbf{P}}_\theta\left(y_i = 0 \mid x_i\right)}\right)}_{\text{Log odds}}$$

Implications?

$$\phi(x_i)^T\theta = 0 \quad \overset{\exp(0)=1}{\Rightarrow} \quad \hat{\mathbf{P}}_\theta\left(y_i = 1 \mid x_i\right) = \hat{\mathbf{P}}_\theta\left(y_i = 0 \mid x_i\right)$$

$$\phi(x_i)^T\theta > 0 \quad \overset{\exp(\epsilon)>1}{\Rightarrow} \quad \hat{\mathbf{P}}_\theta\left(y_i = 1 \mid x_i\right) > \hat{\mathbf{P}}_\theta\left(y_i = 0 \mid x_i\right)$$

$$\phi(x_i)^T\theta < 0 \quad \overset{\exp(-\epsilon)<1}{\Rightarrow} \quad \hat{\mathbf{P}}_\theta\left(y_i = 1 \mid x_i\right) < \hat{\mathbf{P}}_\theta\left(y_i = 0 \mid x_i\right)$$

for any positive ϵ

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

Definition

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

Substituting the above result:

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

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

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

Defn. of σ

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

Definition

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

Defn. of σ

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

Simplified Loss Minimization Problem

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

The Loss for Logistic Regression

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

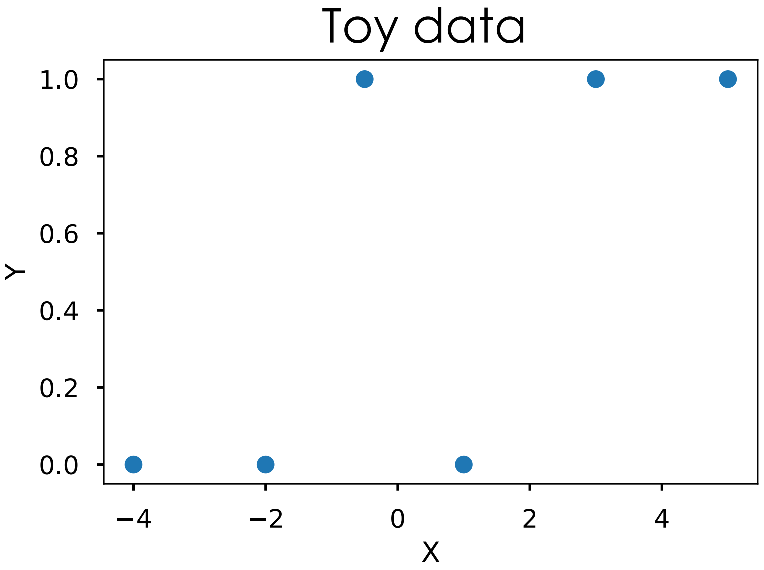
$$\arg\min_{\theta} -\frac{1}{n}\sum_{i=1}^{n}\left(y_i\phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)\right)$$

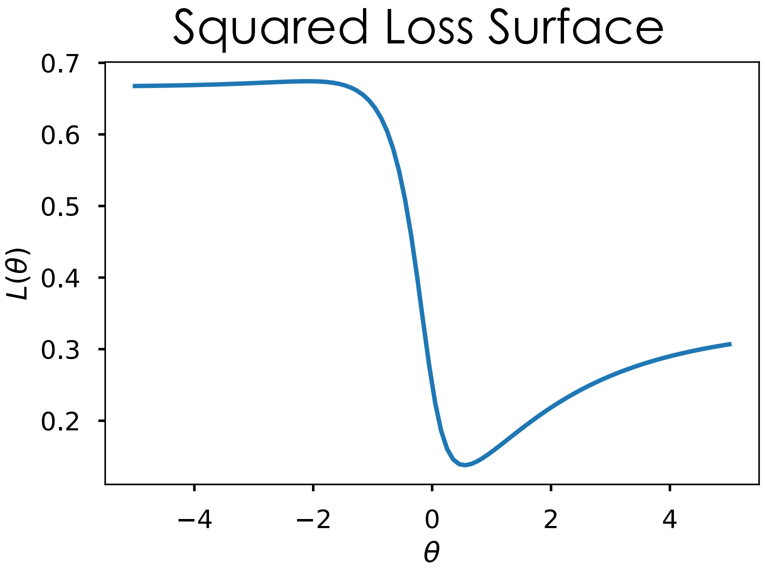
  - Equivalent to (derived from) **minimizing the KL divergence**
  - Also equivalent to **maximizing the log-likelihood of the data** … (not covered in DS100 this semester)

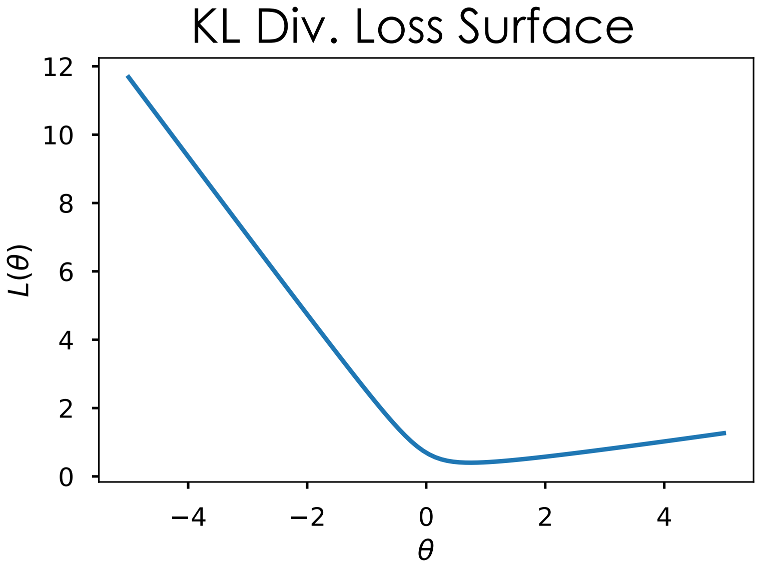
Is this loss function reasonable?

Convexity Using Pictures

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







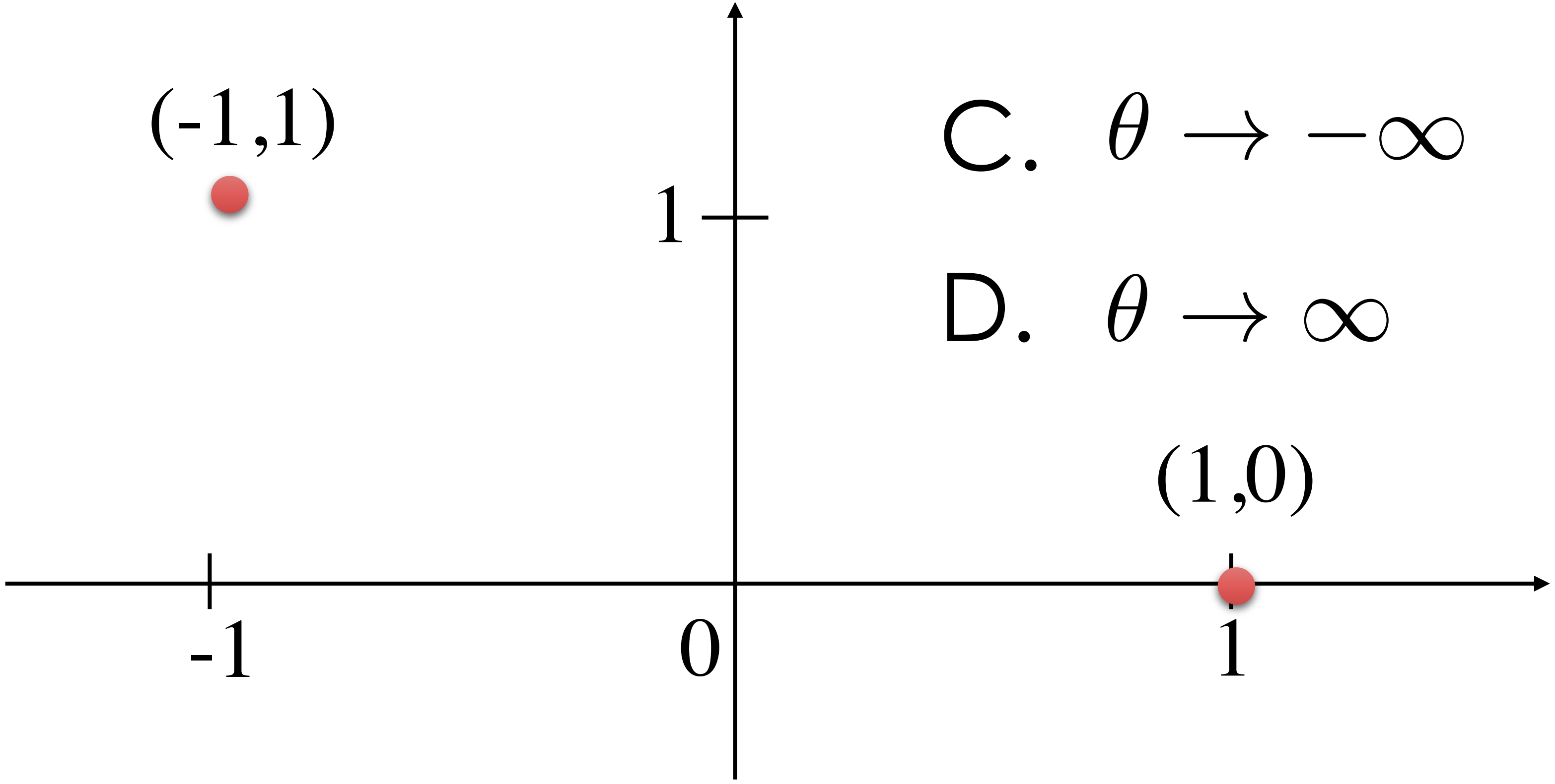
What is the value of θ?

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

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

Assume: $\phi(x) = x$

The Data

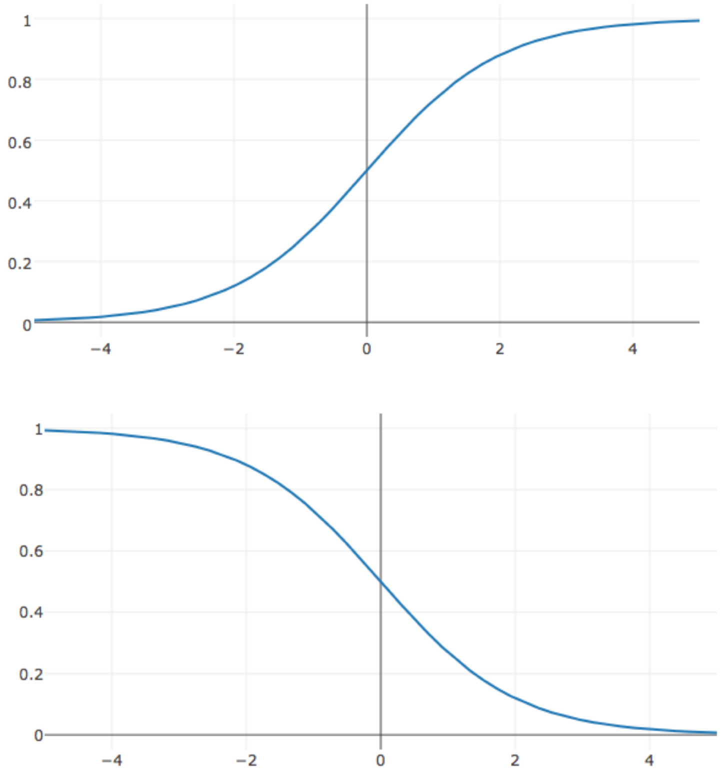


A. $\theta = -1$

B. $\theta = 1$

C. $\theta \rightarrow -\infty$

D. $\theta \rightarrow \infty$



What is the value of θ?

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

Assume: $\phi(x) = x$

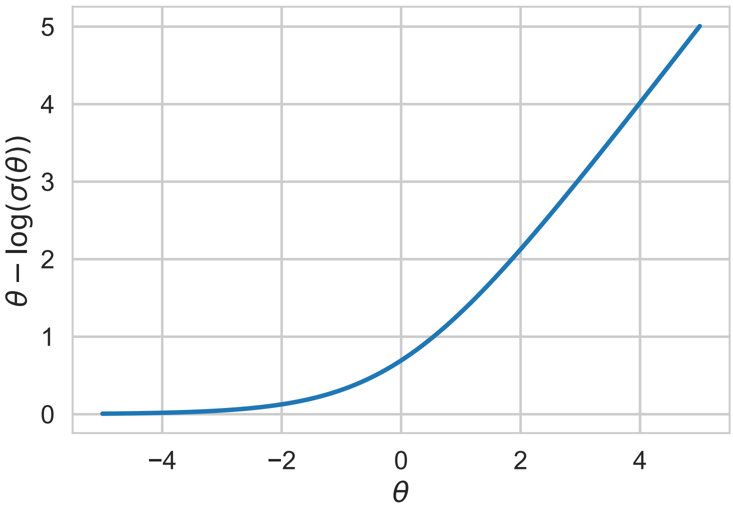
For the point (-1,1):

$$y_i\phi(x_i)^T = -1$$

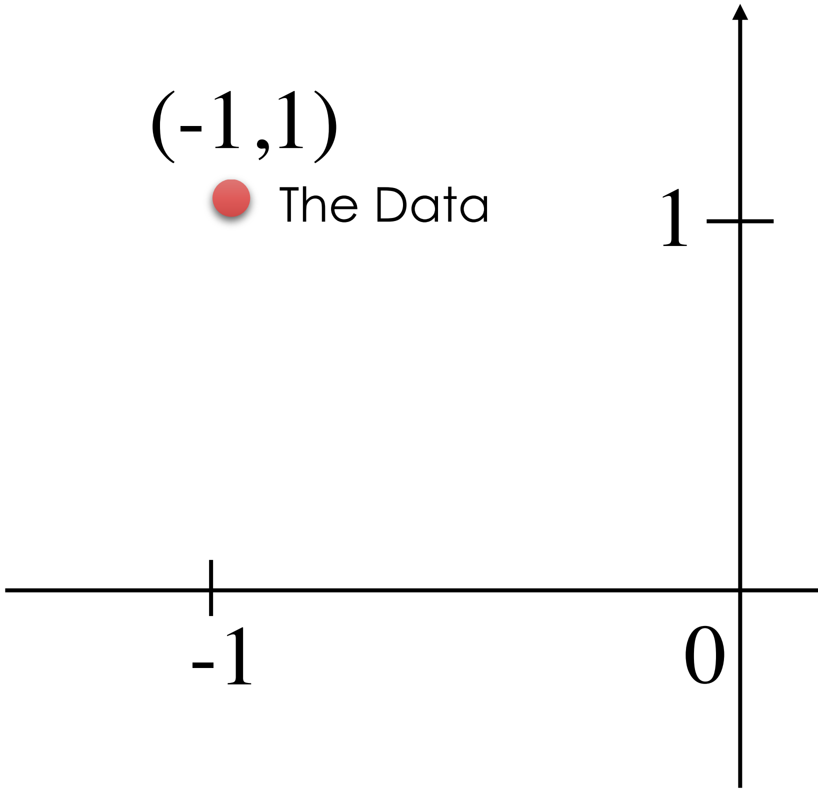
$$-\phi(x_i)^T = 1$$

Objective:

$$\theta - \log\left(\sigma\left(\theta\right)\right)$$



$$\theta \to -\infty$$



What is the value of θ?

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

For the point (-1,1): $\theta - \log\left(\sigma\left(\theta\right)\right)$

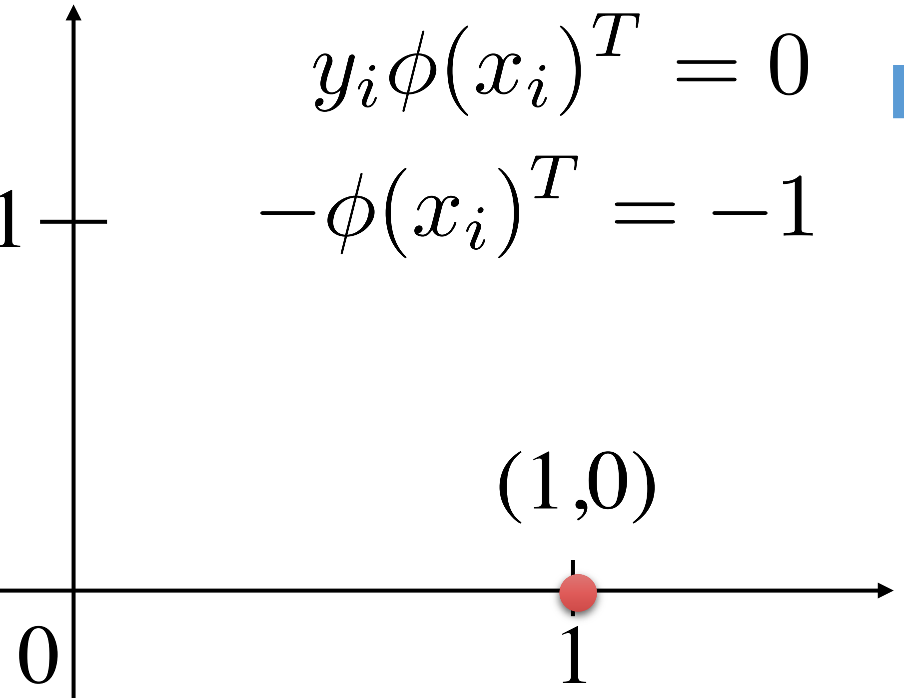
$$\theta \to -\infty$$

Assume: $\phi(x) = x$

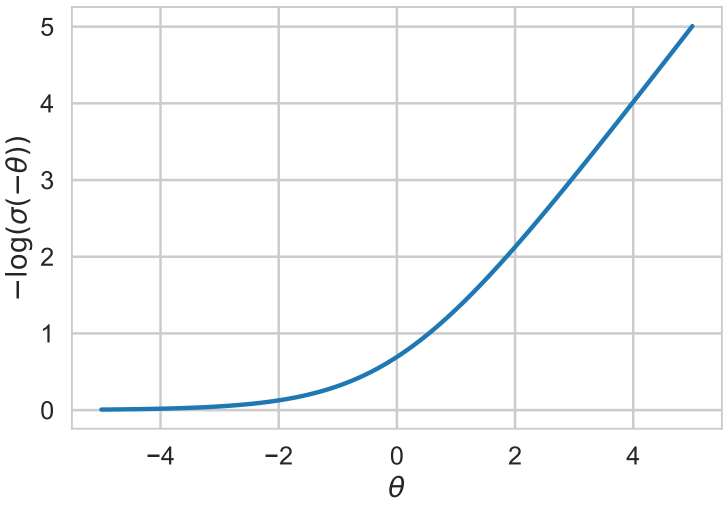
For the point (1, 0):

$$y_i\phi(x_i)^T = 0$$

$$-\phi(x_i)^T = -1$$



➡ $$0 - \log(\sigma(-\theta))$$



$$\theta \to -\infty$$

What is the value of θ?

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

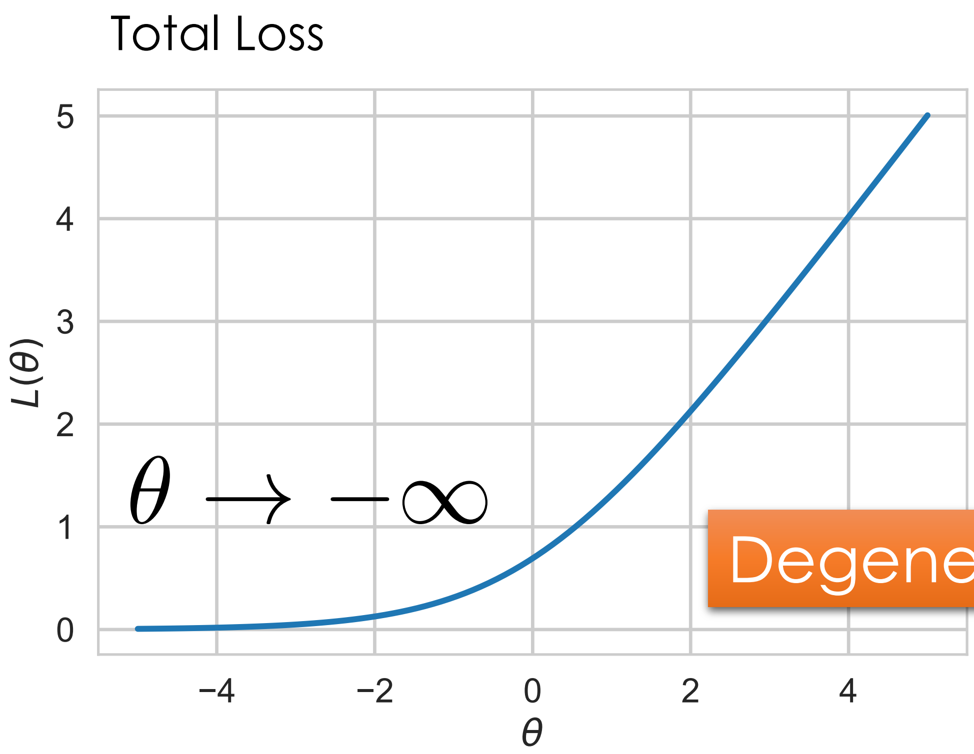
Assume: $\phi(x) = x$

For the point (-1,1): $\theta - \log\left(\sigma\left(\theta\right)\right)$

$$\theta \to -\infty$$

For the point (1, 0): $0 - \log(\sigma(-\theta))$

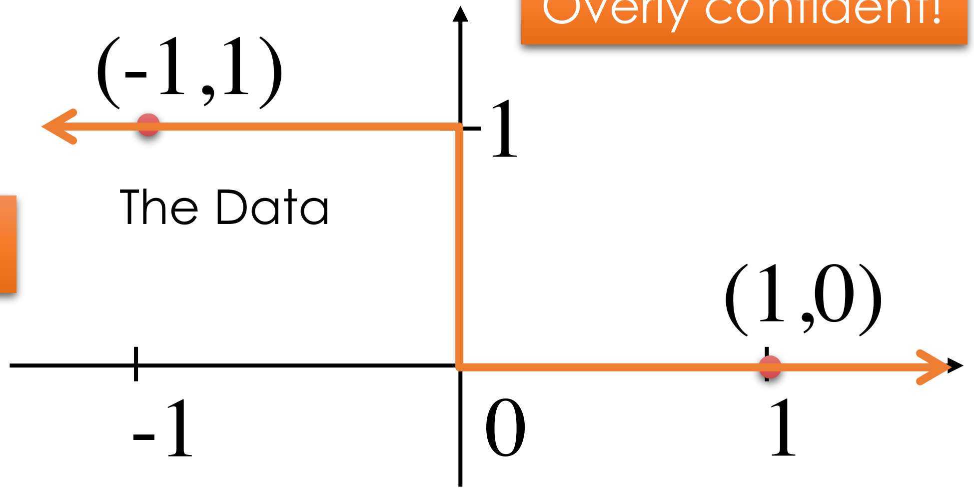
$$\theta \to -\infty$$



$$\theta \to -\infty$$

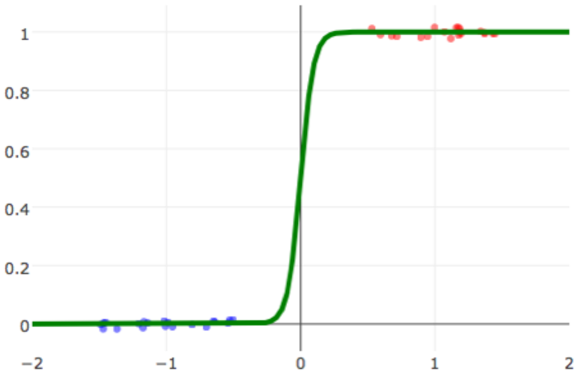
Degenerate Solution!

Overly confident!



Linearly Separable Data

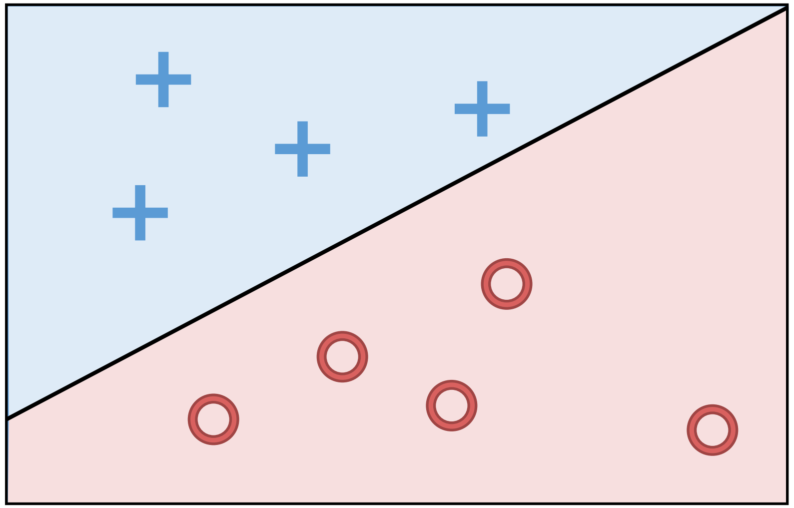
- A classification dataset is said to be linearly separable if there exists a hyperplane that separates the two classes.
- If data is linearly separable, logistic regression requires regularization



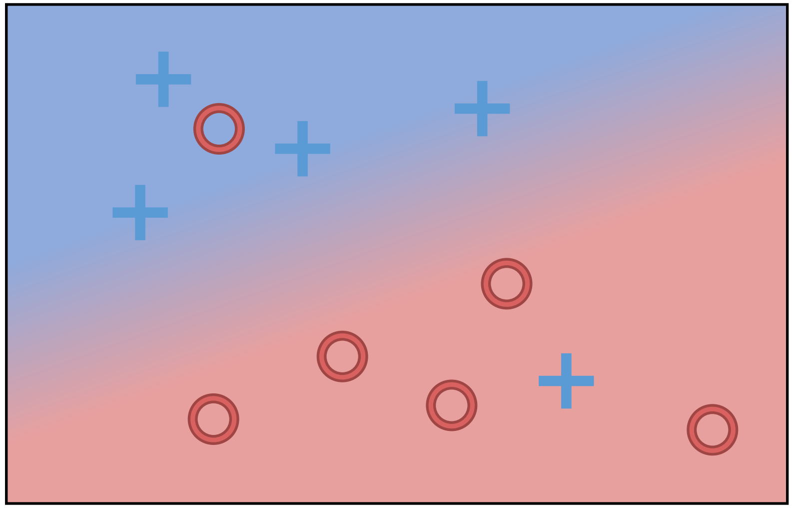
Weights go to infinity!

Solution?

Linearly Separable Data



Not Linearly Separable Data

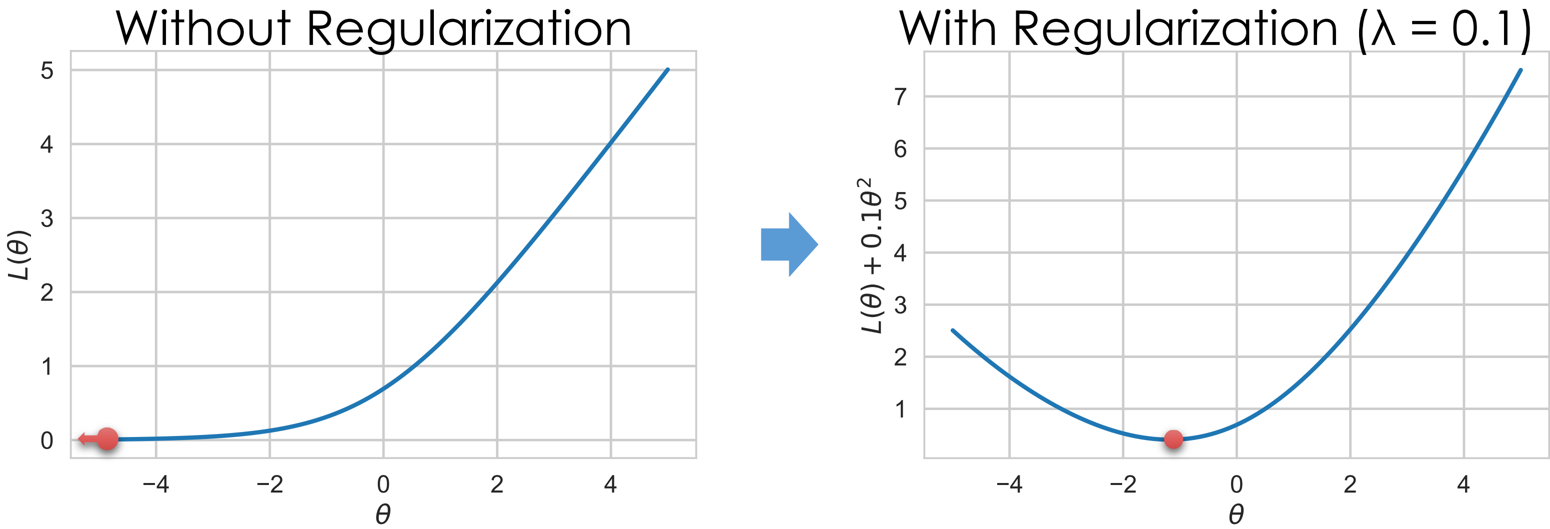


Adding Regularization to Logistic Regression

$$\arg\min_{\theta} -\frac{1}{n}\sum_{i=1}^{n}\left(y_i\phi(x_i)^T\theta + \log\left(\sigma\left(-\phi(x_i)^T\theta\right)\right)\right) + \lambda\sum_{j=1}^{d}\theta_j^2$$

- Prevents weights from diverging on linearly separable data

Earlier Example



Minimize the Loss

Logistic Loss Function

- Average KL divergence (simplified)

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

- Take Derivative:

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

- Average KL divergence (simplified)

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

- Take Derivative:

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

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

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

- Take Derivative:

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

Useful Identity

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

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

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

- Take Derivative:

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

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

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

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

Logistic Loss Function

- Average KL divergence (simplified)

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

- 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:

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

- **$\rho(\tau)$** 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:

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

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

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:

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

- What if we approximated the gradient by looking at a few random points:

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

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:

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

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

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

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

For τ from 0 to convergence:

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

Stochastic Gradient Descent

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

For τ from 0 to convergence:

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

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

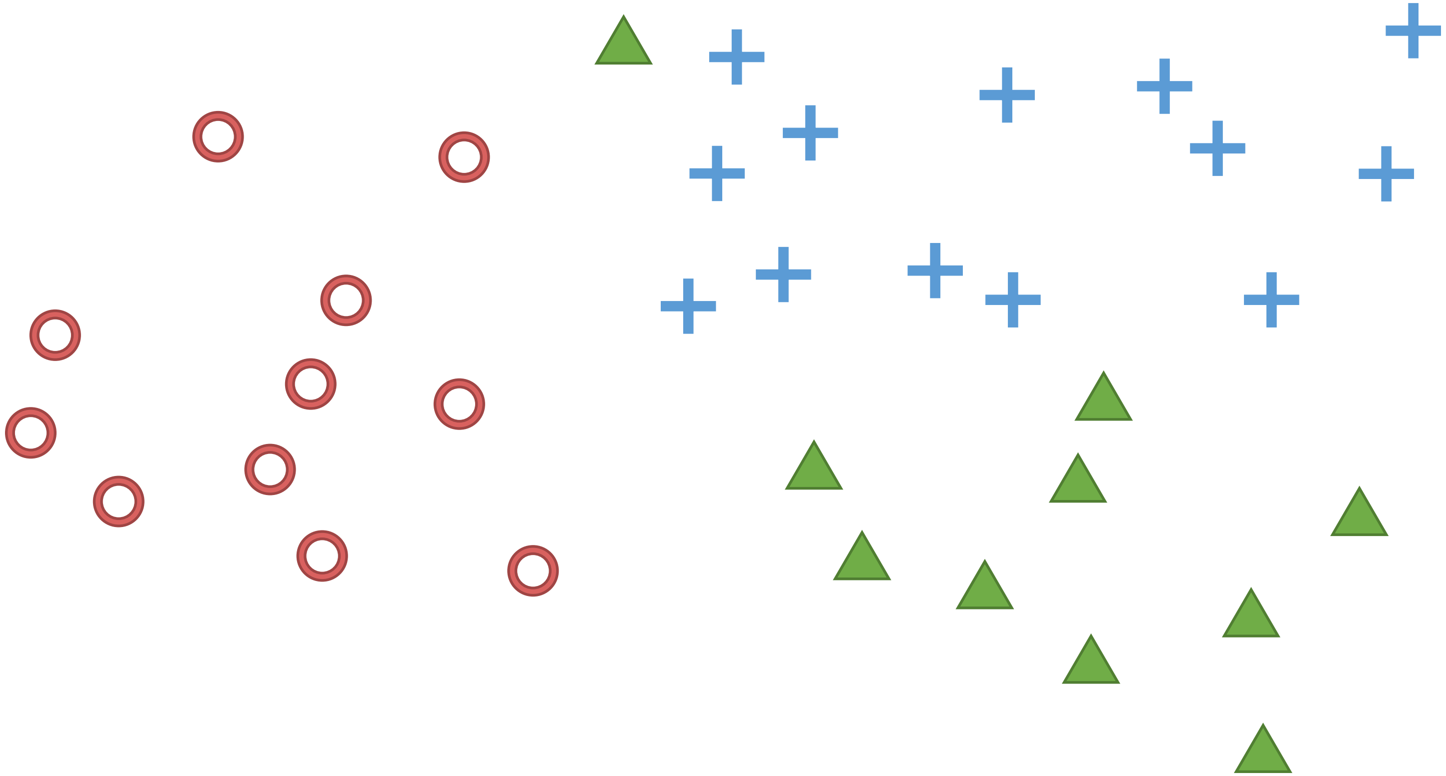
Very Similar Algorithms

Assuming Decomposable Loss Functions

Python Demo!

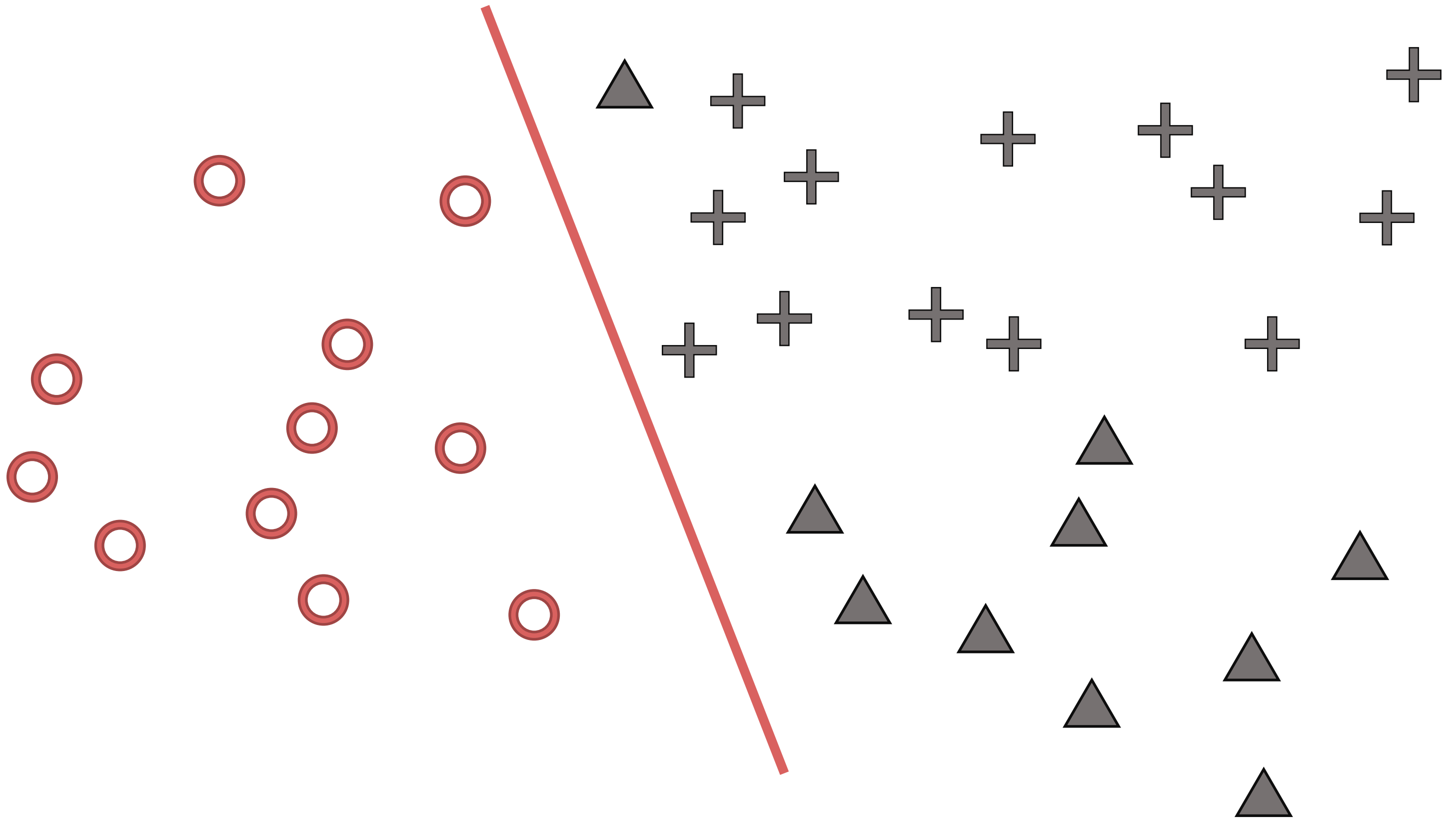
Multiclass (more than 2) Classification

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



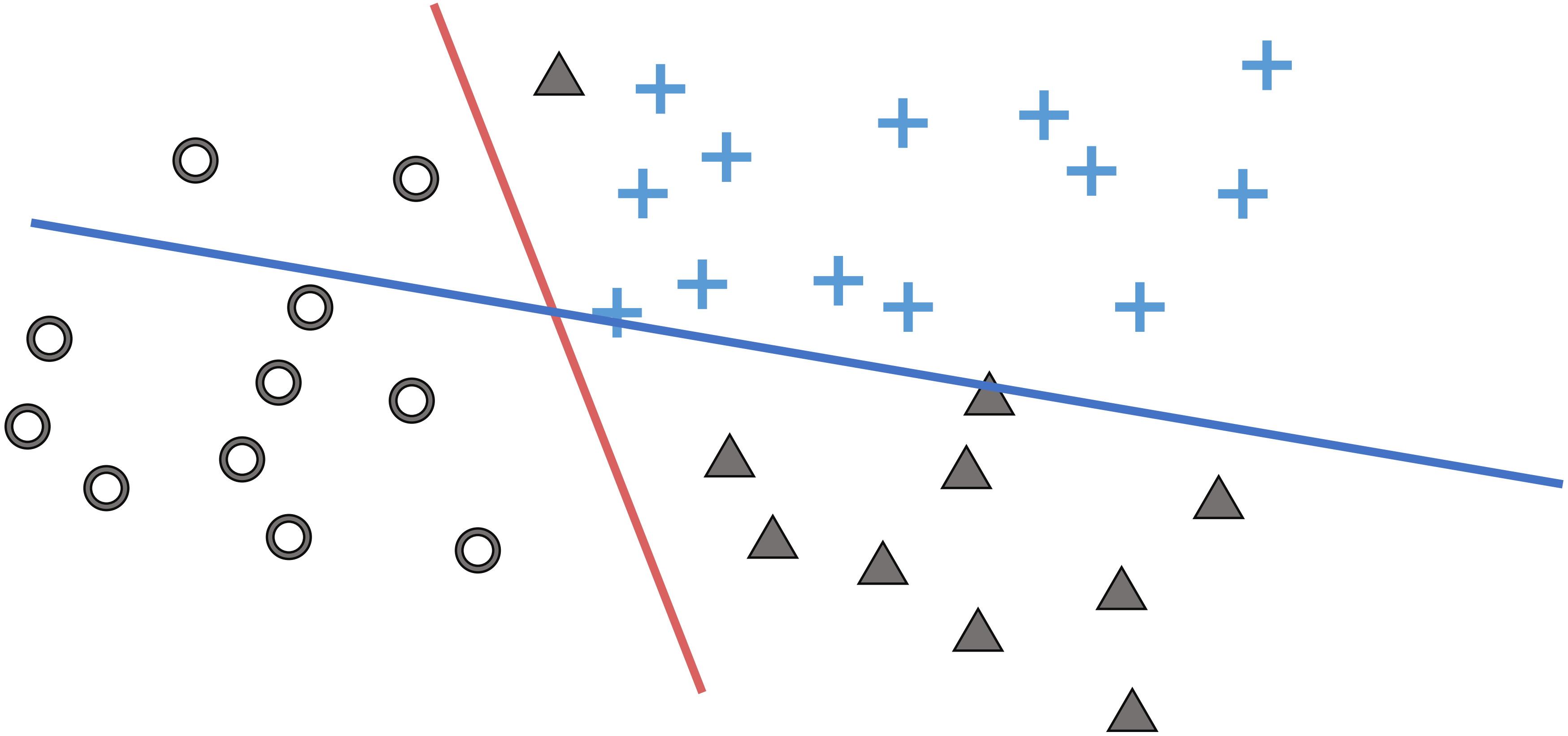
Multiclass (more than 2) Classification

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



Multiclass (more than 2) Classification

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



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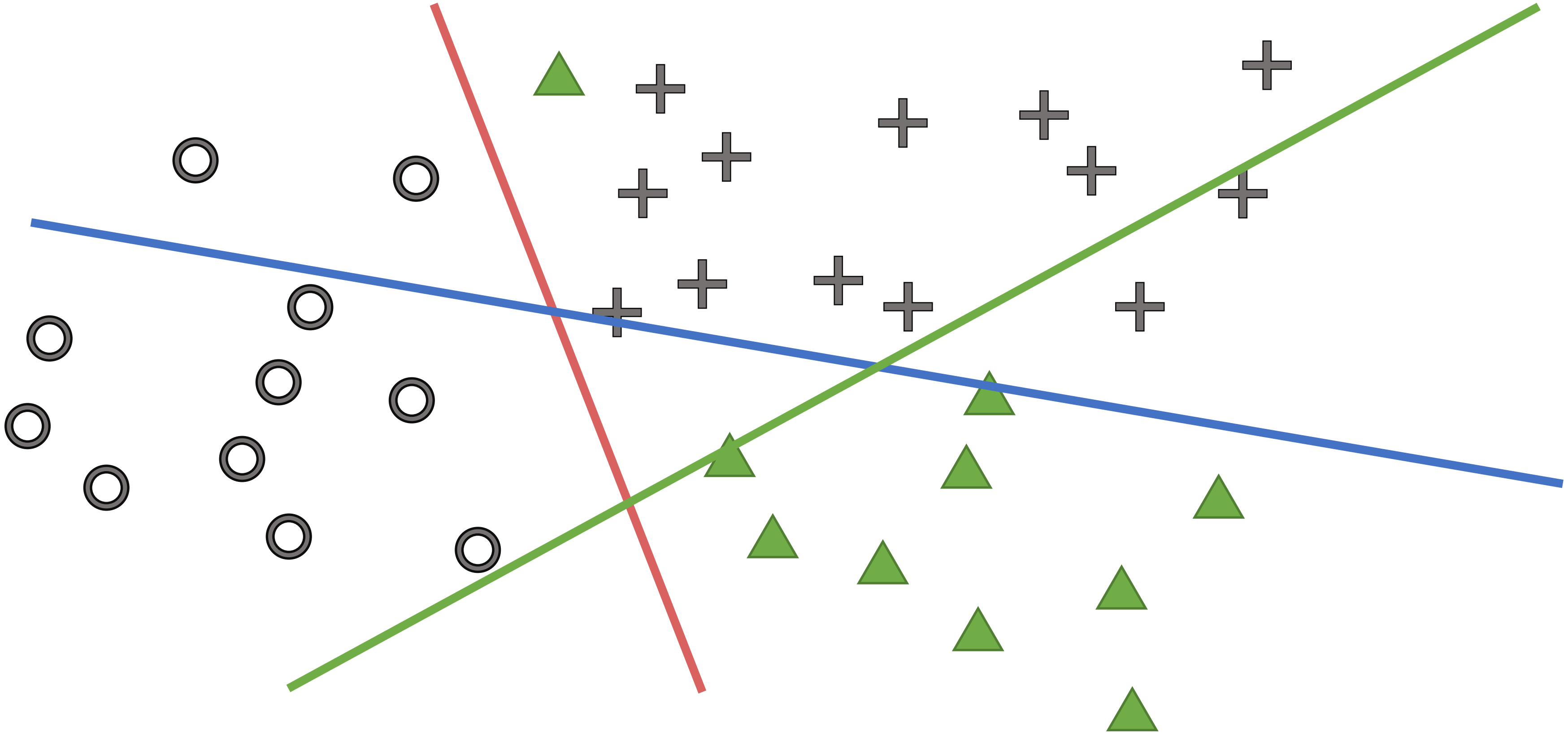

Multiclass (more than 2) Classification

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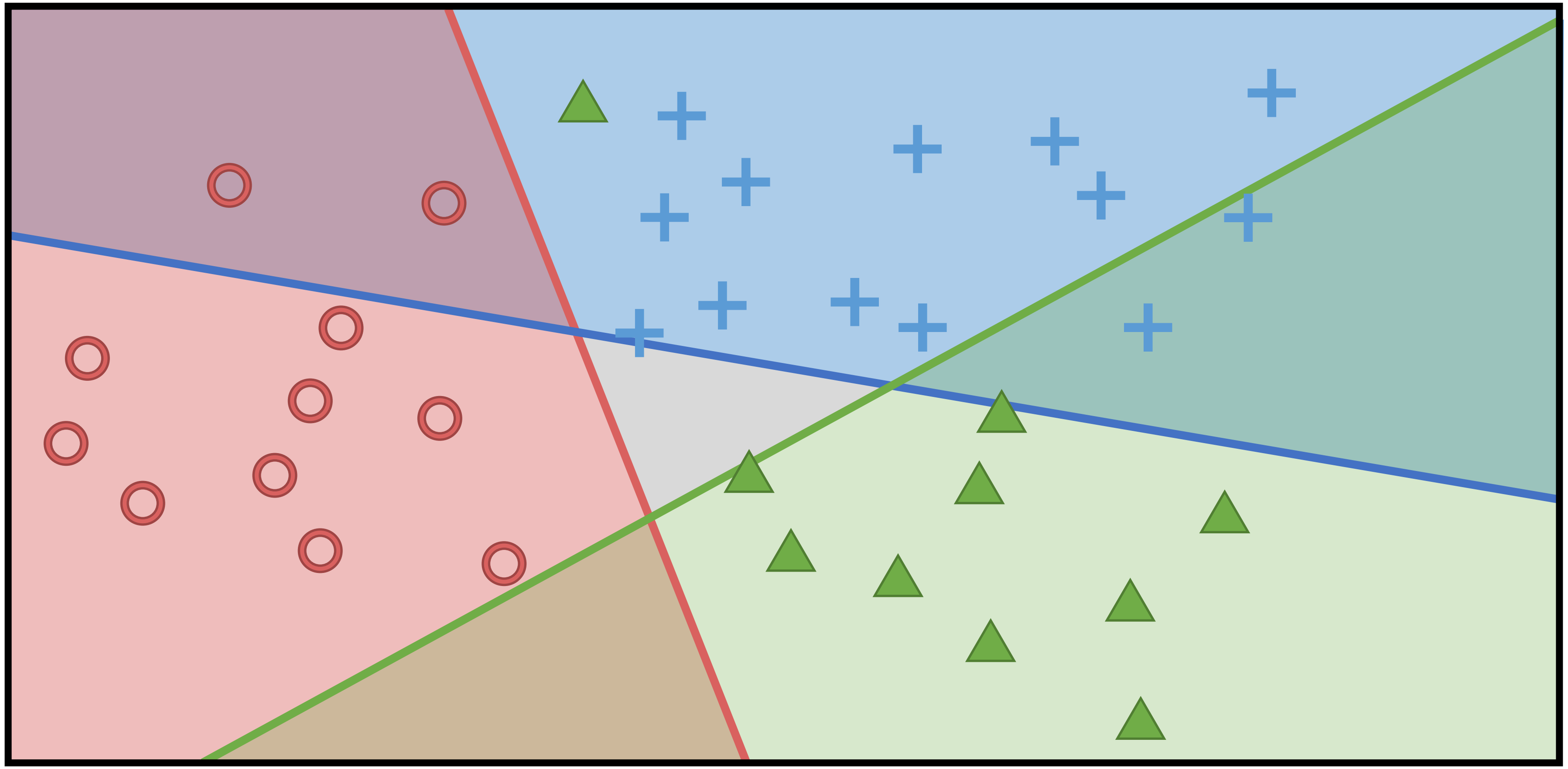
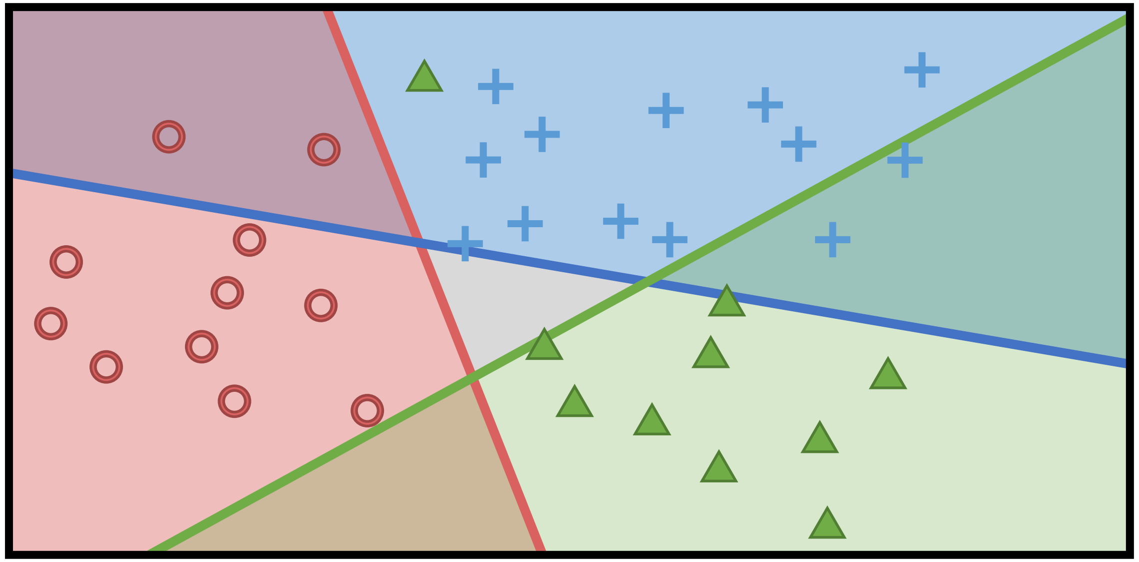


Multiclass (more than 2) Classification

- **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

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

- 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

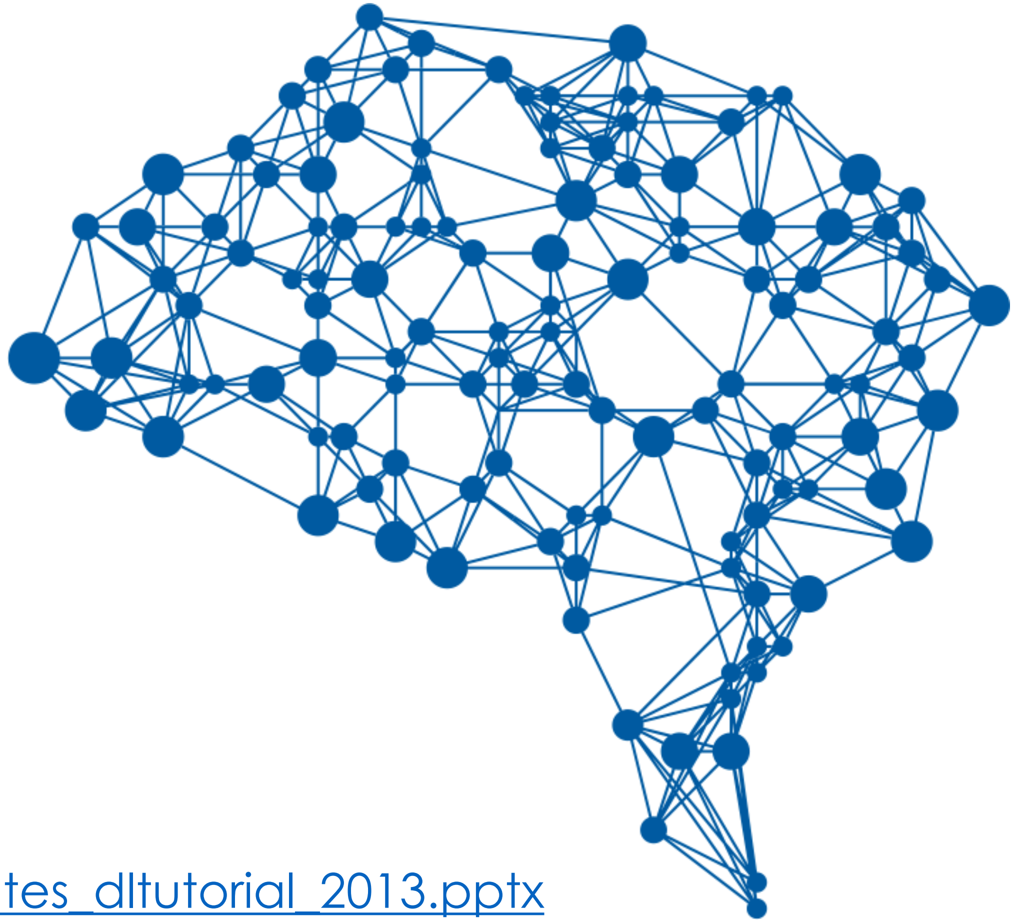
$$\mathbf{P}\left(y = k \,|\, x\right) = 1 - \sum_{j=1}^{K} \mathbf{P}\left(y = j \,|\, x\right)$$

  - Often use k parameters + regularization to address “redundancy”.

Python Demo!

Deep Learning Overview

Bonus Material



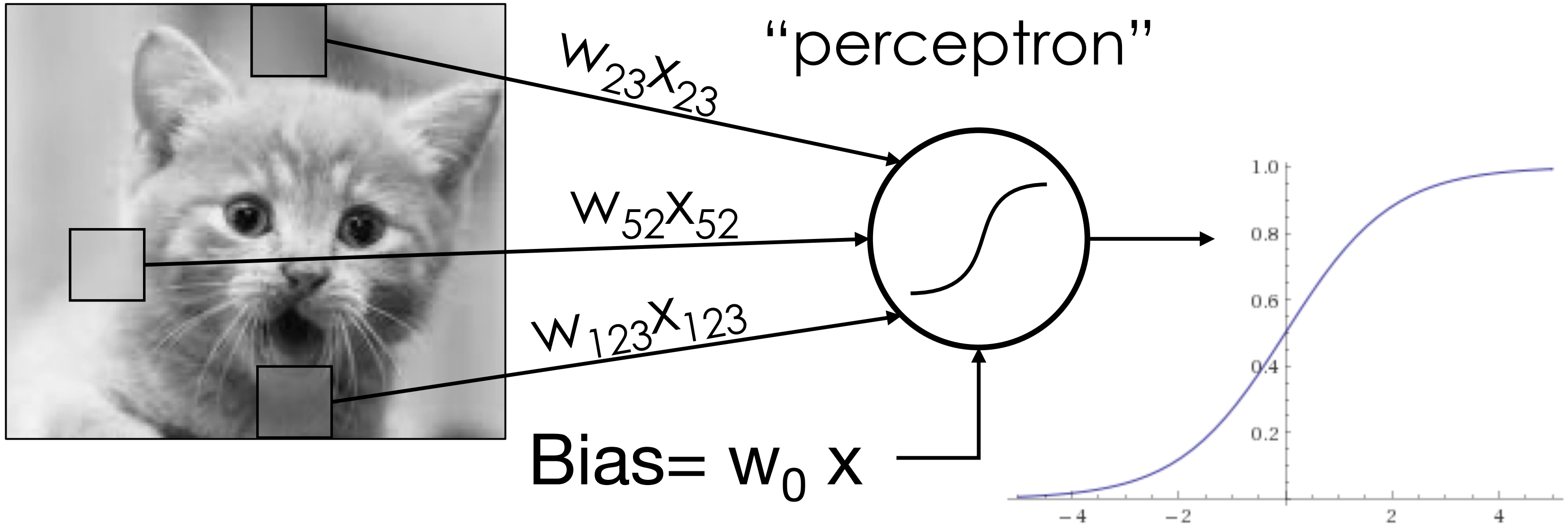
Borrowed heavily from excellent talks by:

- **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: $\sigma(u) = \dfrac{1}{1+\exp(-u)}$

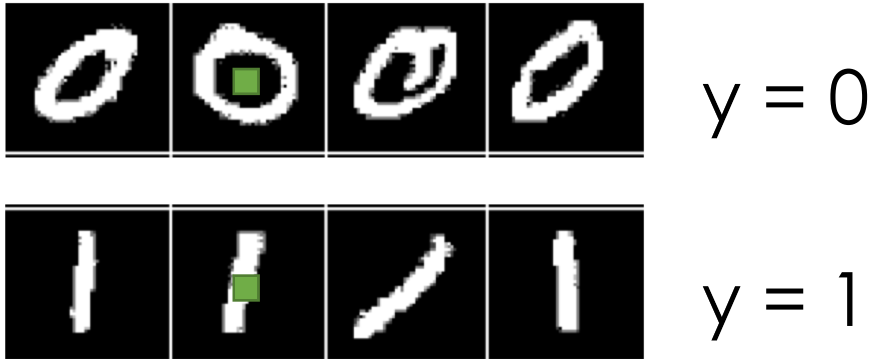
$$f_w(x) = \sigma\left(w^T x\right) = \sigma\left(\sum_{j=1}^{d} w_j x_j\right) = P(y = 1 \,|\, x)$$

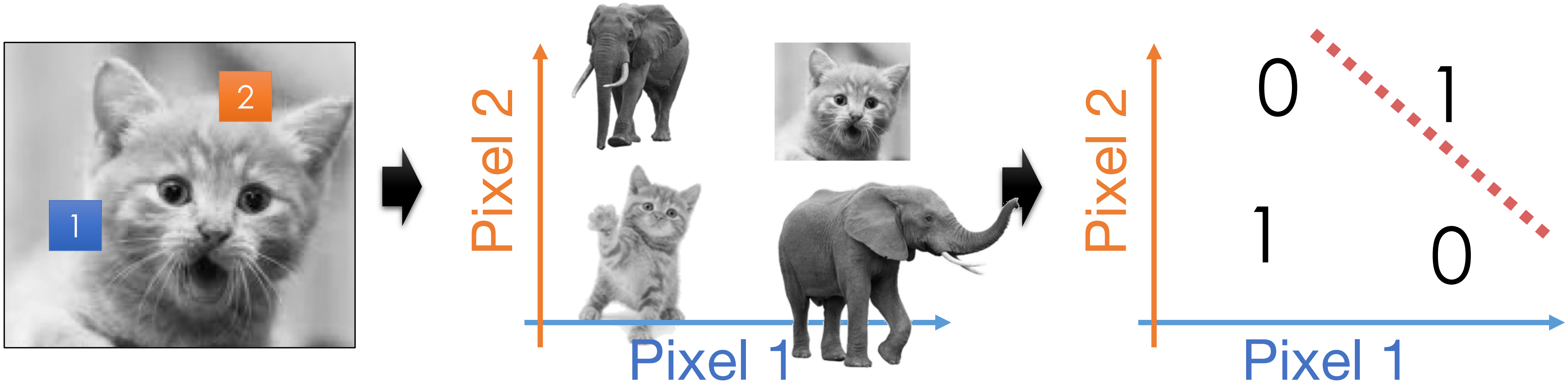


Neuron “fires” if weighted sum of input is greater than zero.

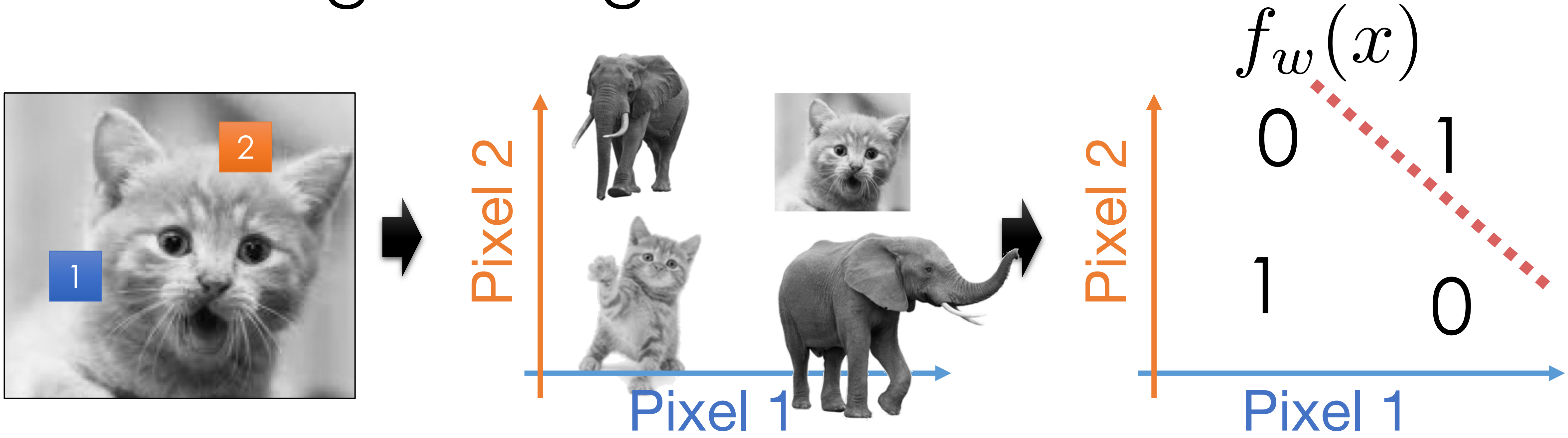
Logistic Regression: Strengths and Limitations

- 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

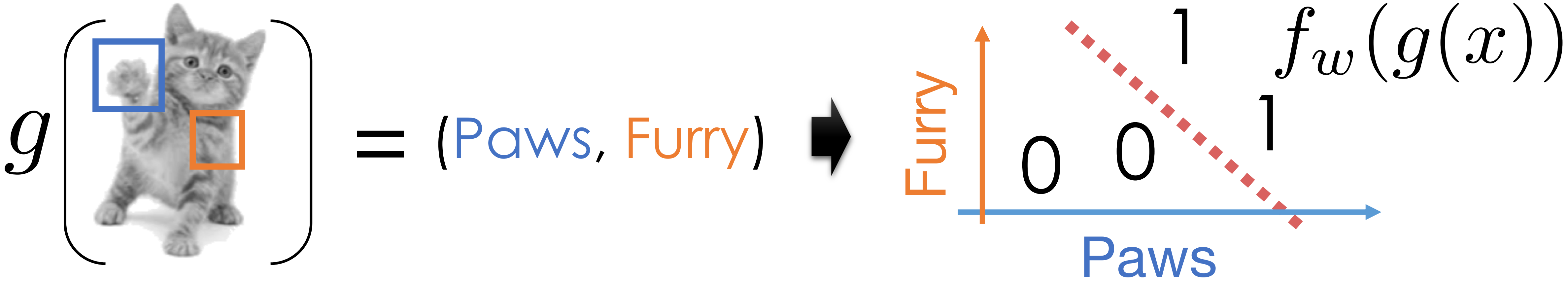




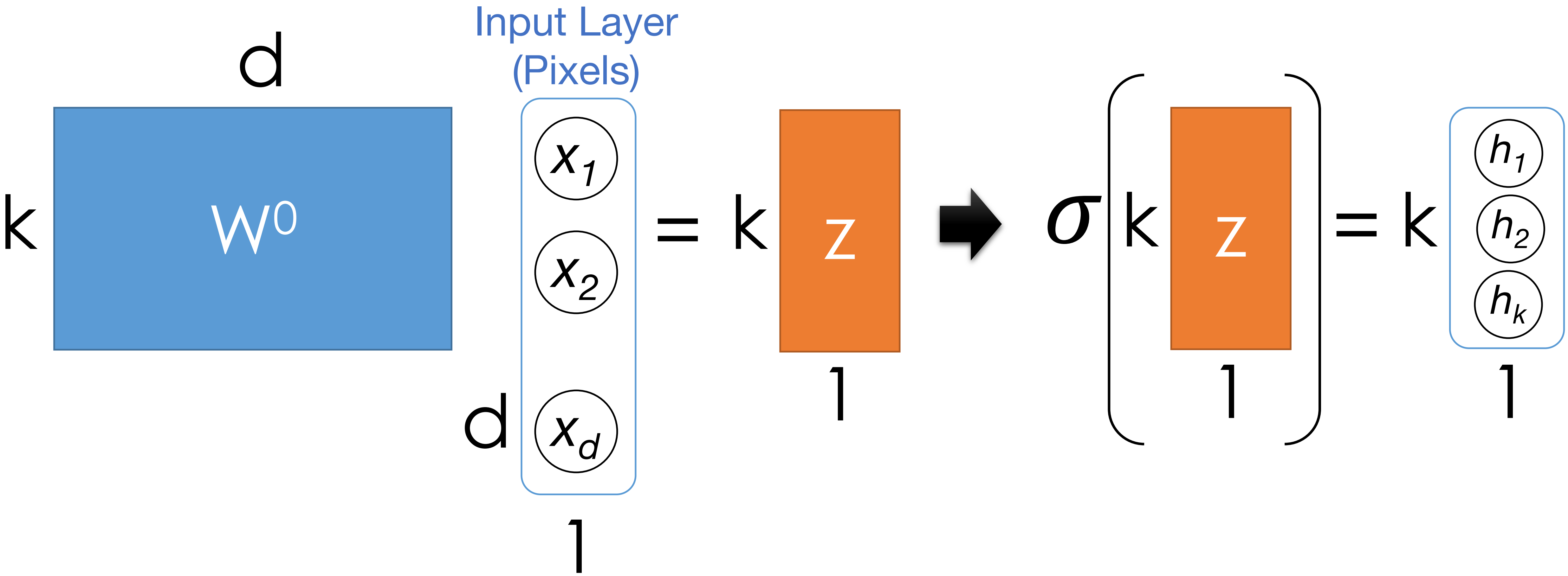
Feature Engineering



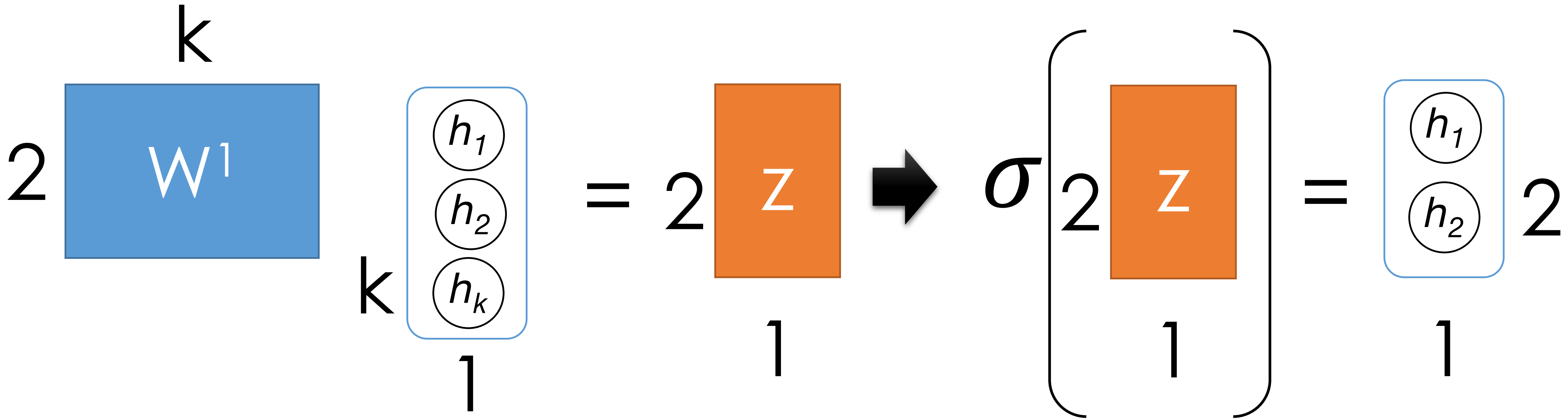
- Rather than use raw **pixels build/train feature functions:**



Composition Linear Models and Nonlinearities



Composition Linear Models and Nonlinearities

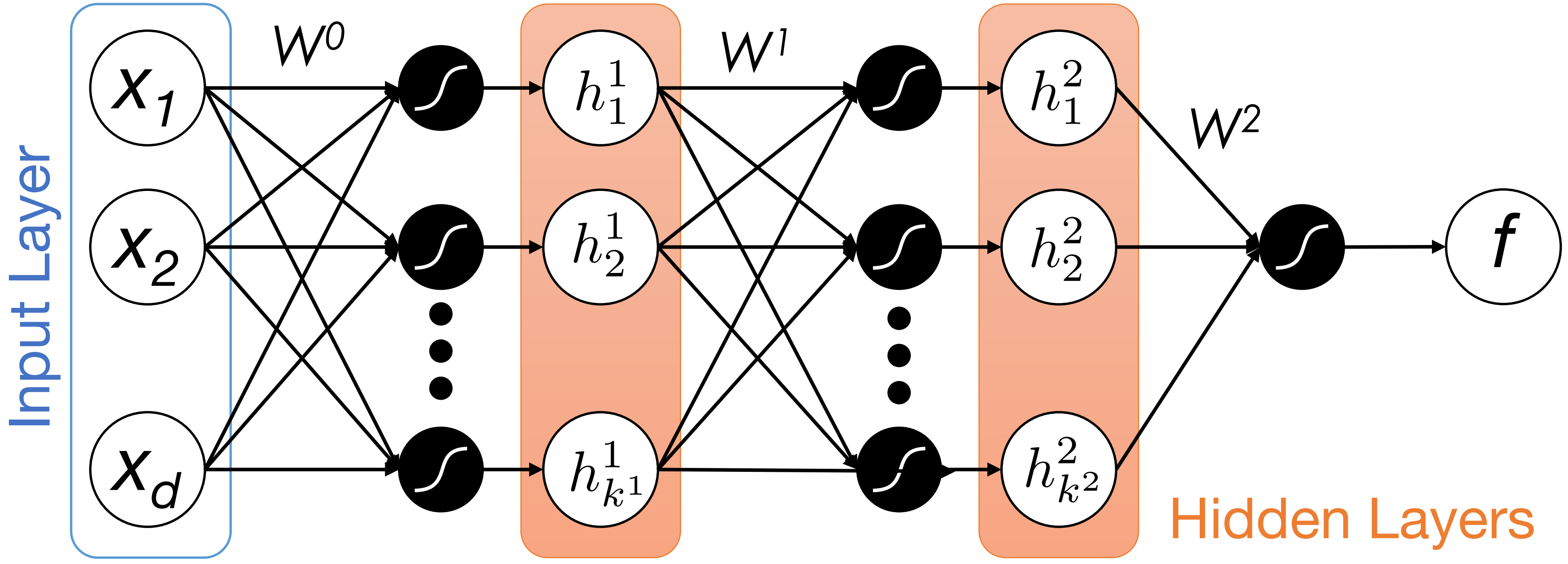


Neural Networks

- Composing "perceptrons"

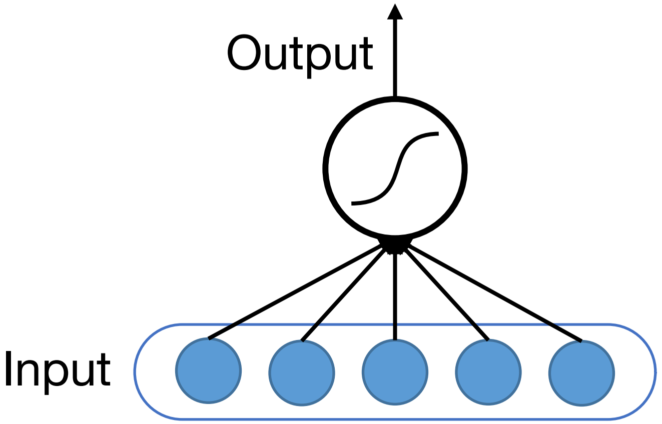
$$x \rightarrow \sigma(W^0 x) \rightarrow h^1 \rightarrow \sigma(W^1 h^1) \rightarrow h^2 \rightarrow \sigma(W^2 h^2) \rightarrow f$$

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

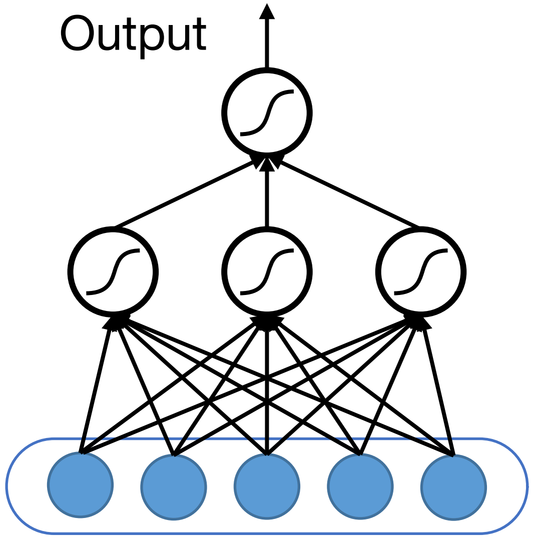


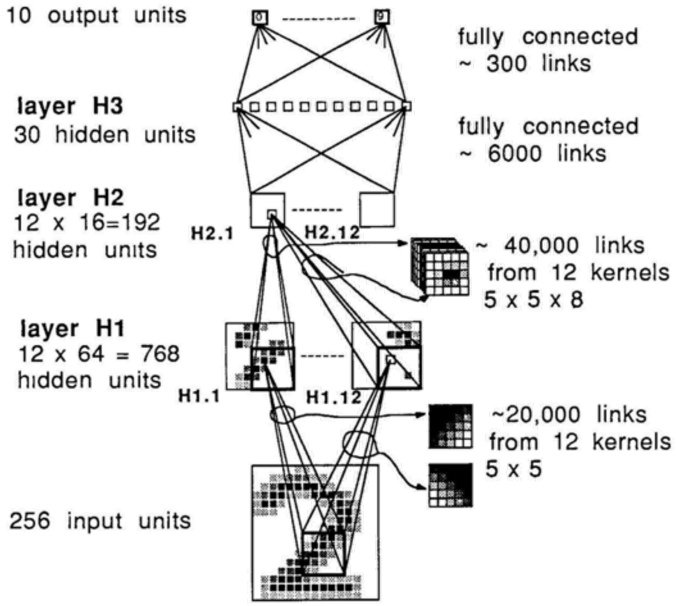
Deep Learning →Many hidden layers

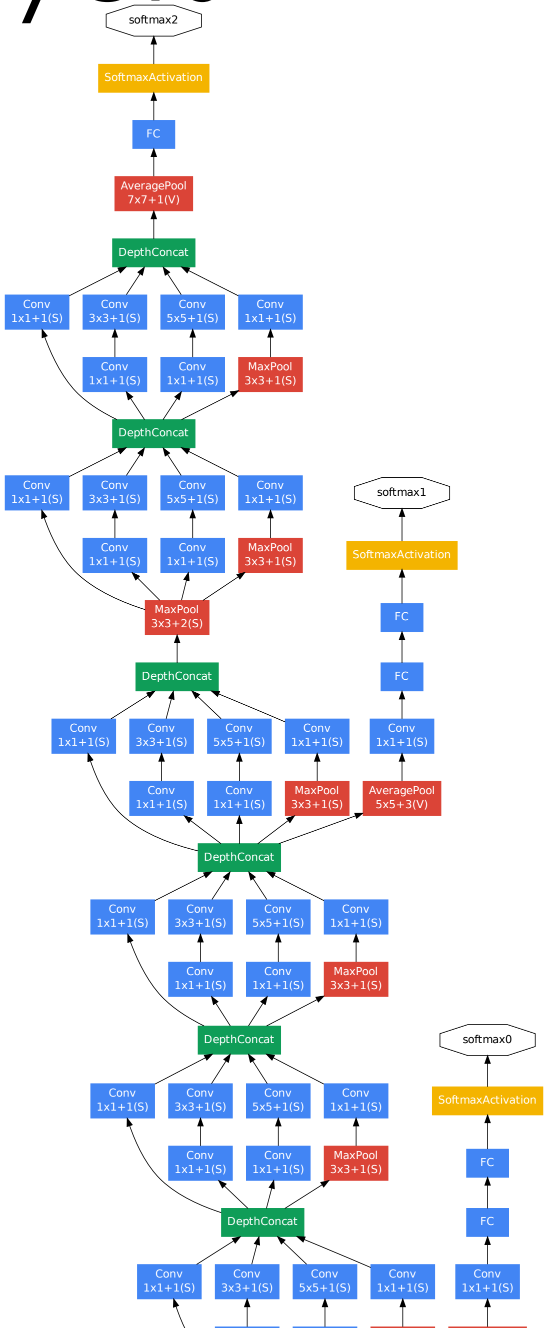
…



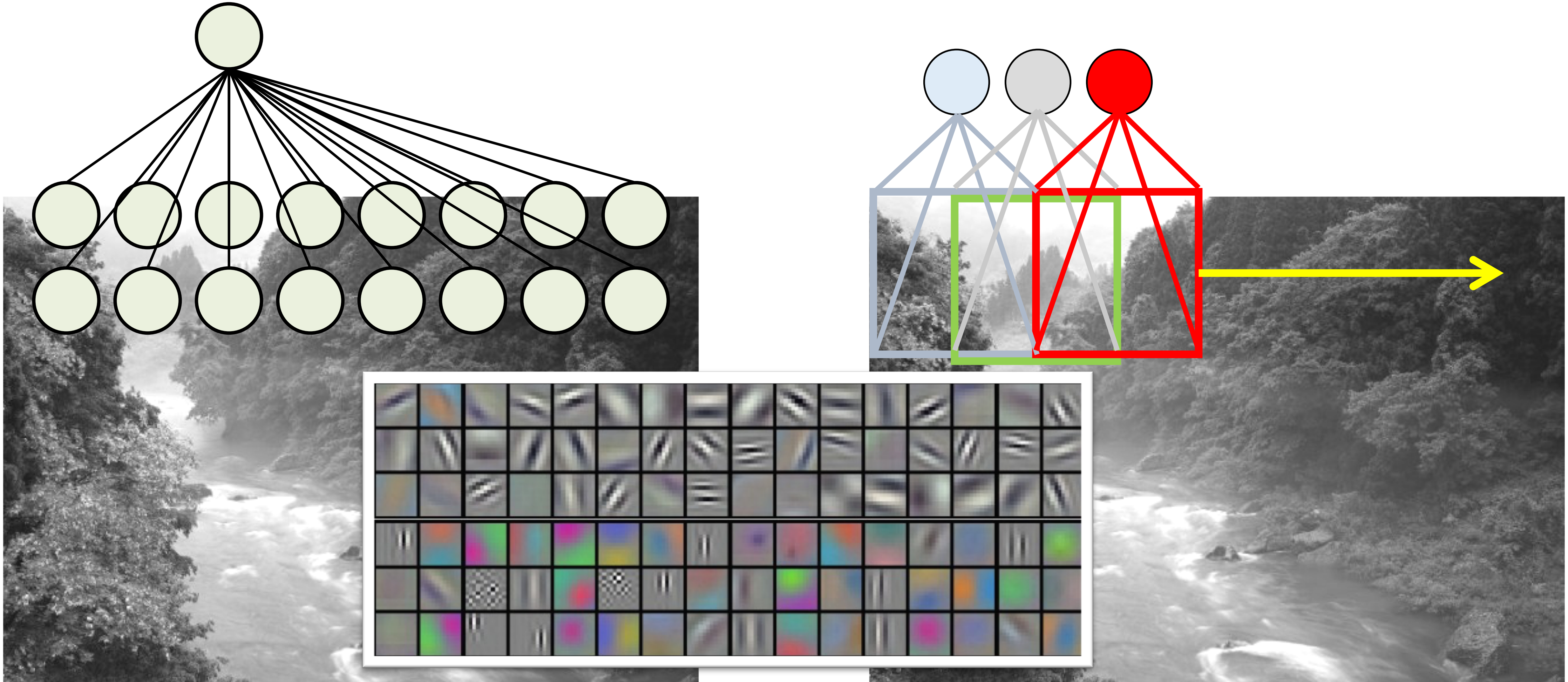
Logistic Regression



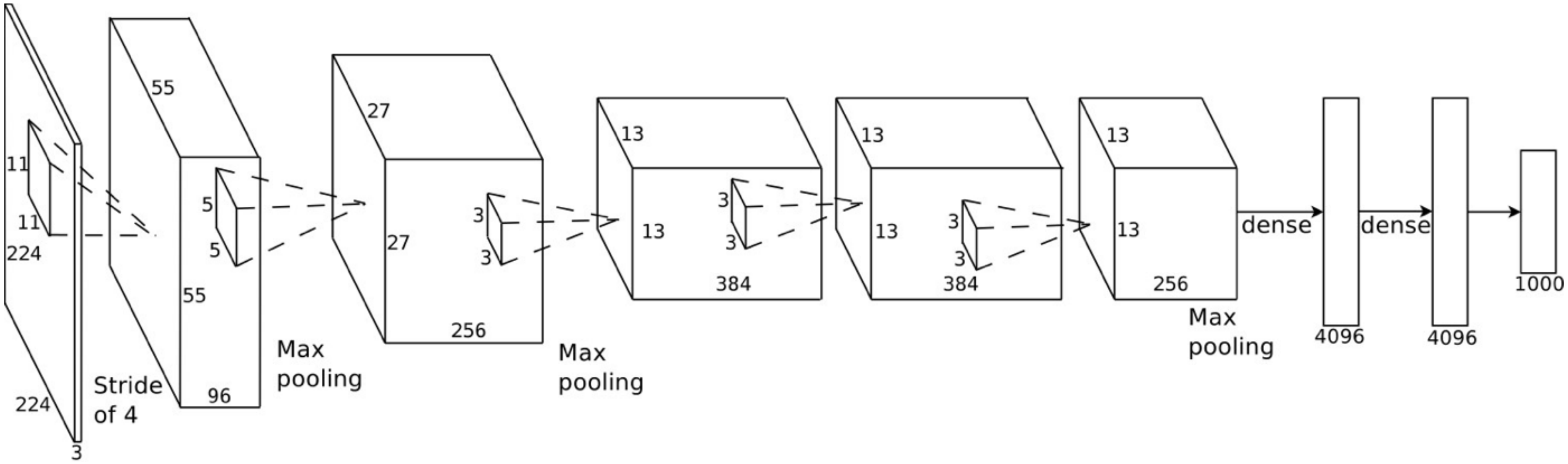




Convolutional Neural Networks: Exploiting Spatial Sparsity

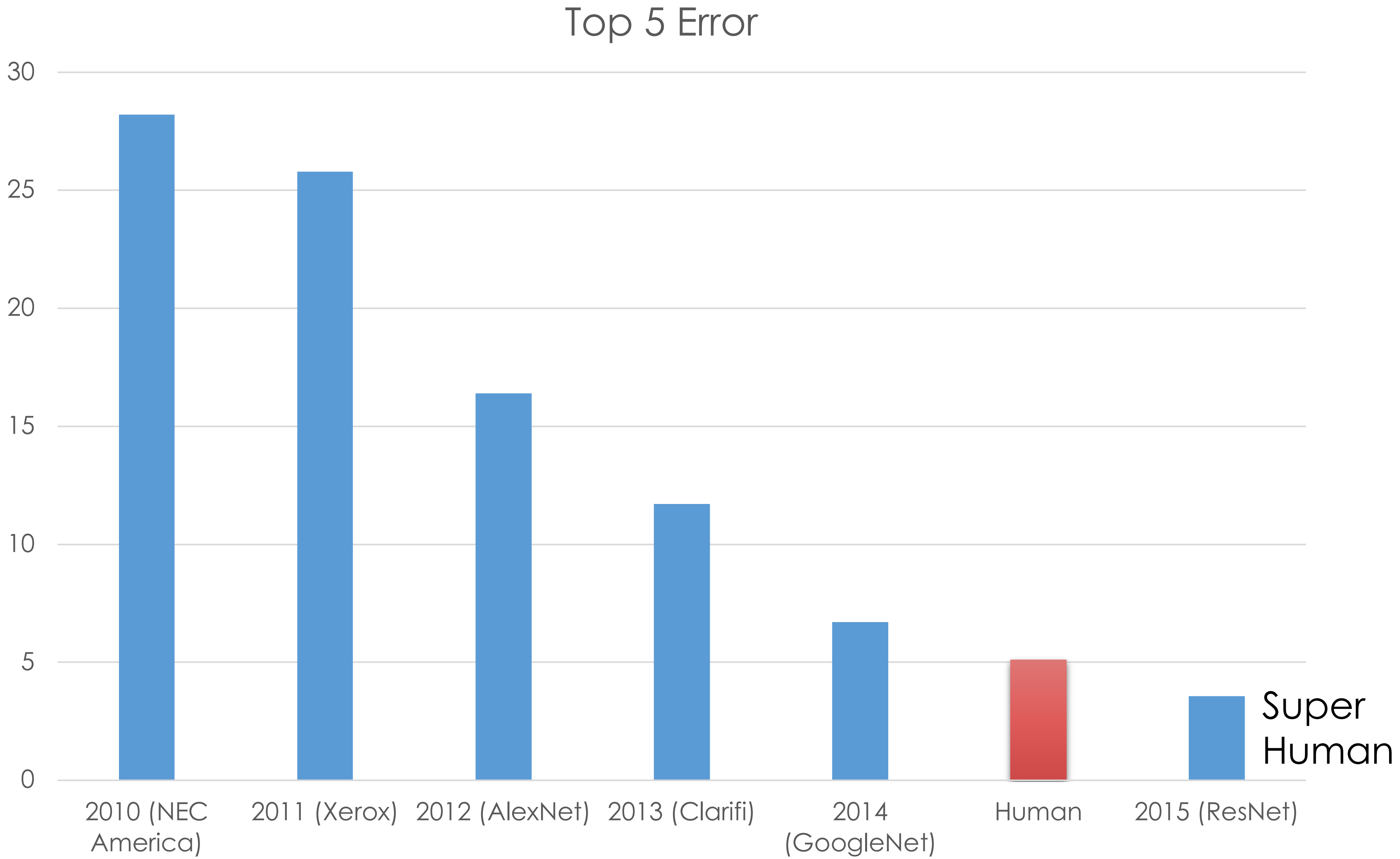


Example: AlexNet (Krizhevsky et al., NIPS 2012)

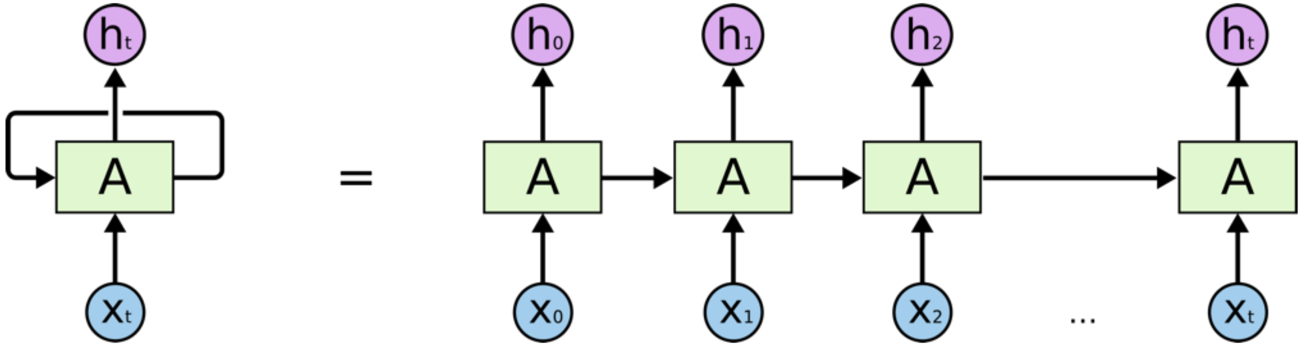


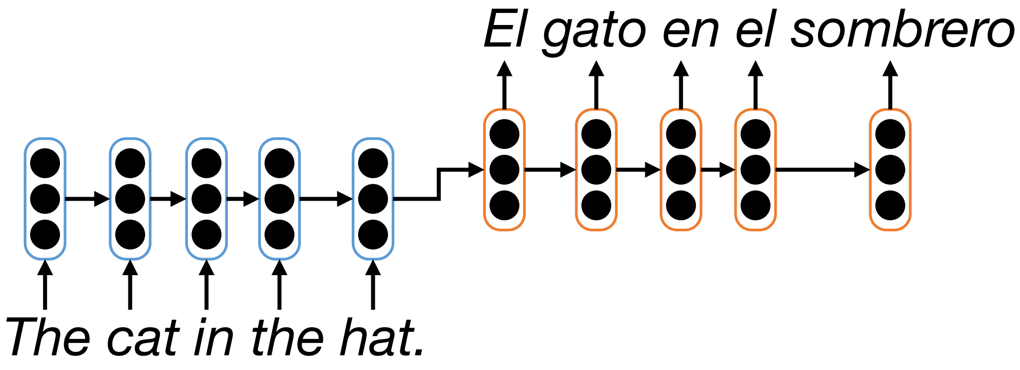
- ➢ Introduced in 2012, significantly outperformed state-of-the-art (top 5 error of 16% compared to runner-up with 26% error)

Improvement on ImageNet Benchmark



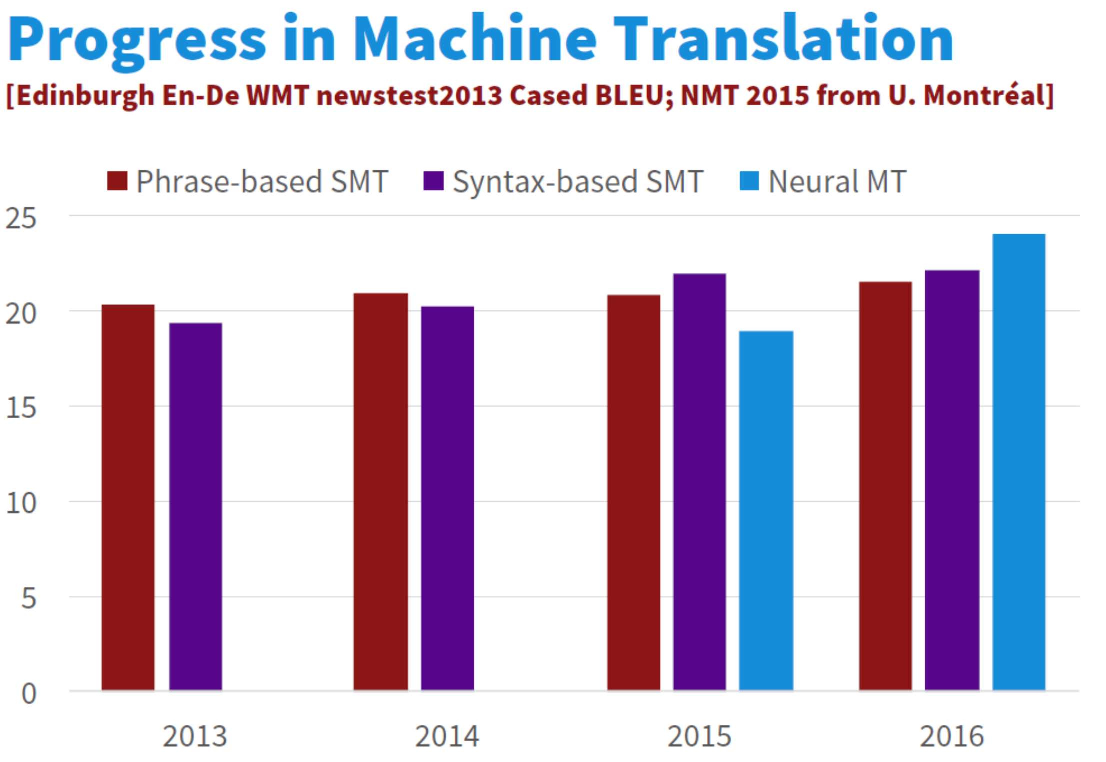
Recurrent Neural Networks:
Modeling Sequence Structure





- ➢ input + previous output → new output
- ➢ State of the art in modeling sequential data
  - ➢ speech recognition and machine translation

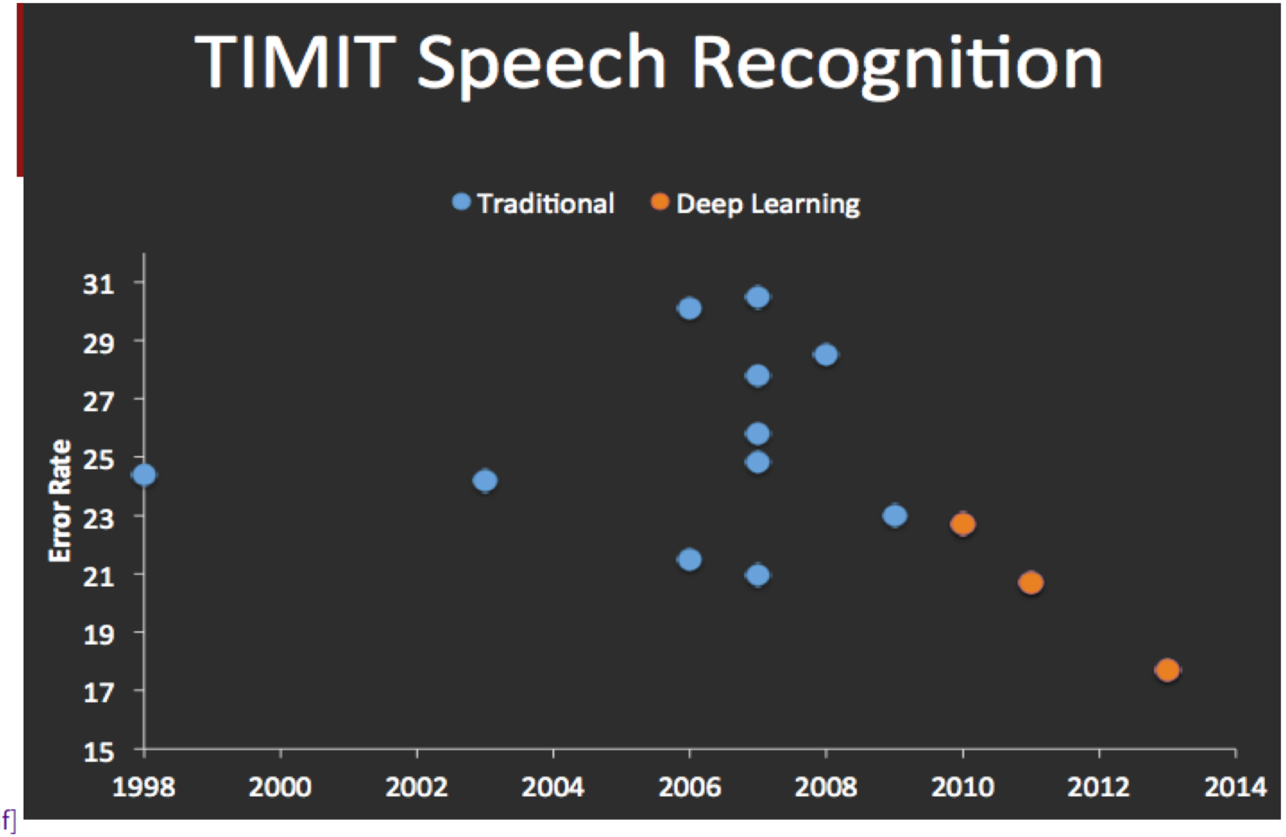
Improvements in Machine Translation & Automatic Speech Recognition



Progress in Machine Translation

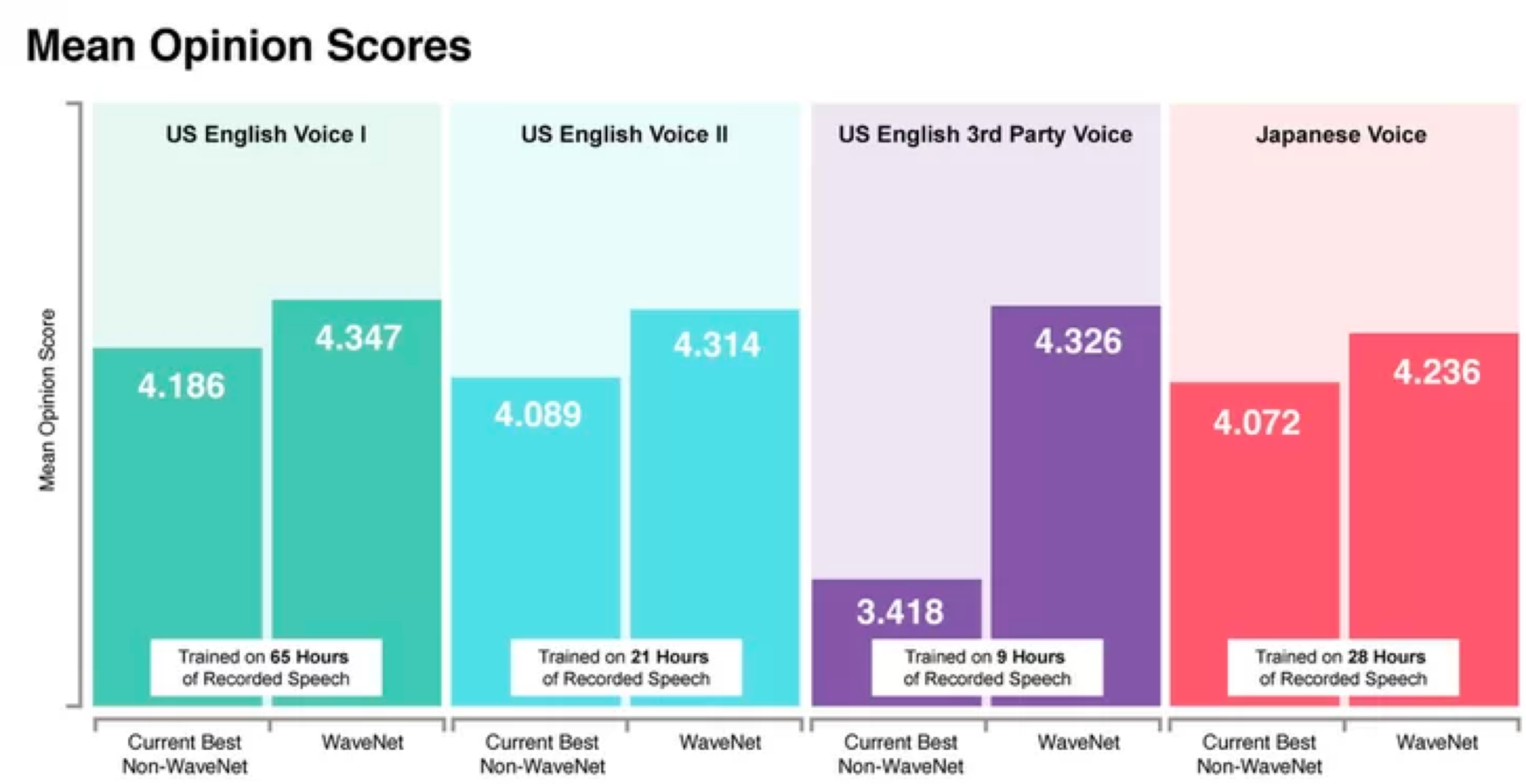
[Edinburgh En-De WMT newstest2013 Cased BLEU; NMT 2015 from U. Montréal]

From [Sennrich 2016, http://www.meta-net.eu/events/meta-forum-2016/slides/09_sennrich.pdf]



TIMIT Speech Recognition

State of the art in Text to Speech (TTS)



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/