Introduction to Regression and Machine Learning

CMPT 419/983

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SFU Computing Science

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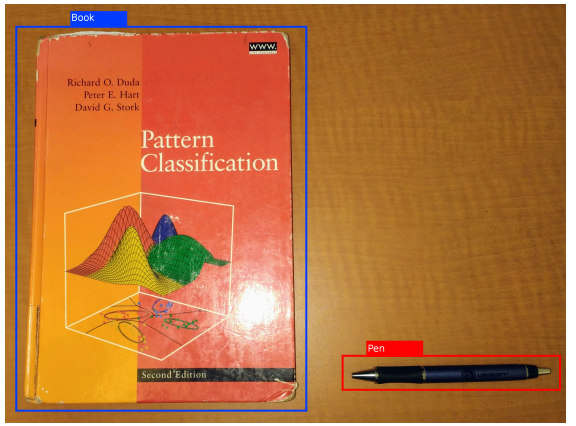
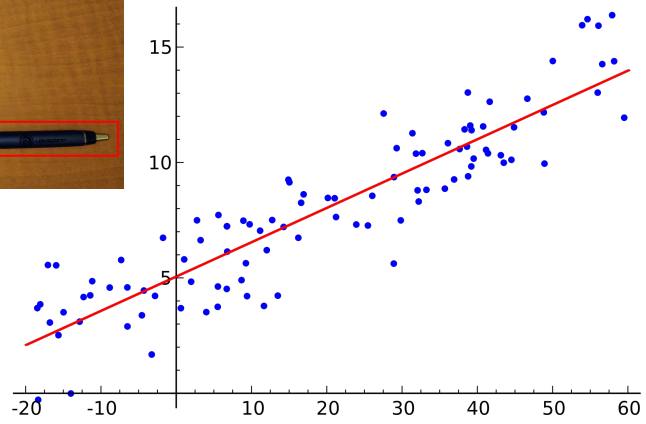
Machine Learning

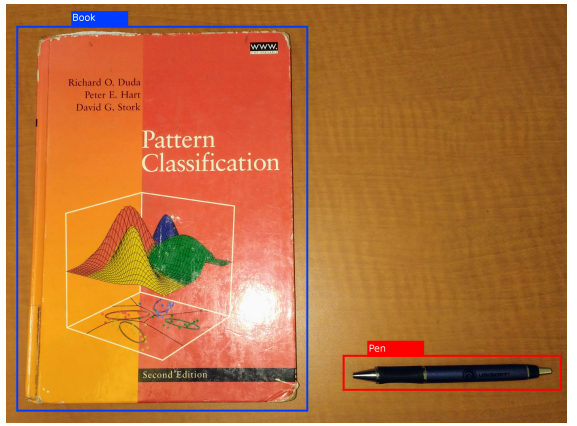


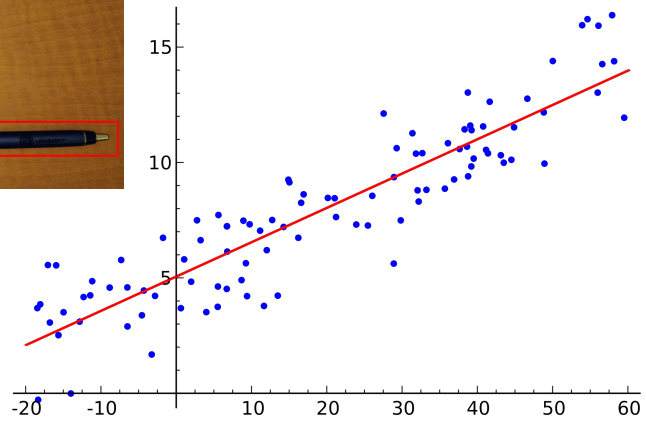


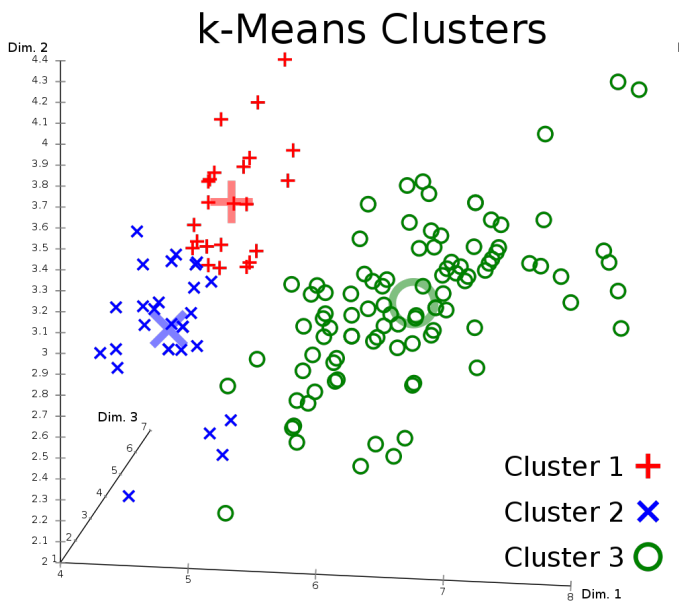
- Goal:
  - Given some inputs x (eg. pixels of an image)
  - Predict some output $y = f(x)$ (eg. object)
- Assumption:
  - During data generation, output y depends on x probabilistically, $y \sim p(x)$
- Procedure:
  - Choose f to be the same type or probability distribution as p (usually unknown)
  - Parametrize f using parameters θ
  - Determine θ that best fits / maximizes the probability of observing data

Machine Learning

- Application of nonlinear optimization
  - Takes advantage of available data
- Supervised learning
  - Regression
  - Classification
- Unsupervised learning
  - Clustering
  - Reinforcement learning







Machine Learning

- Very scalable with additional data
- Requires a lot of data

- Computer vision
- Natural language processing
- Game playing
- Robotics

Outline

- Regression: two perspectives
  - Function fitting
  - Probabilistic interpretation
- Classification
- Neural Networks

Regression

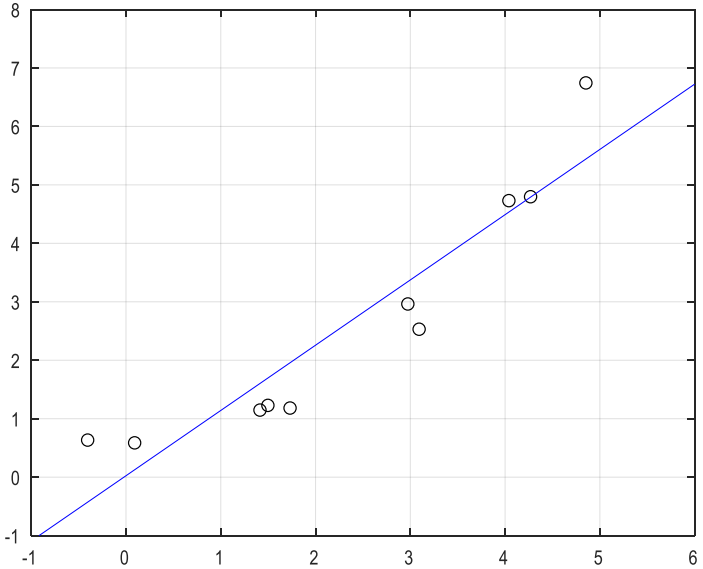
- Given $x \in \mathbb{R}^n$
  - "features", "covariate", "predictors"
- Predict $y \in \mathbb{R}^m$
  - "response", "outputs"
- Learn the function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ such that $y \approx f(x)$
  - f is the model for regression
  - Use data: $\{x_i, y_i\}_{i=1}^N$
- Parametrize the function f using the parameters $\theta \rightarrow y \approx f_\theta(x)$
  - θ and the form of f determines the class of functions in your model
  - Learning $f \rightarrow$ learning parameters θ

Regression

- Supervised learning is regression
  - f_θ is determined through "supervision" by data $\{x_i, y_i\}$
  - We think of data as being "generated in real life" from some probability distribution
- Machine/deep learning is regression using a neural network
  - Neural network (for now): complex f_θ with many components in θ
- Neural networks are hard to analyze, but analyzing regression with simple(r) models provides good intuition

Models for Regression

- Assumed probability distribution from which data is generated



- Simplest model: Linear
  - $y = \theta^\top x + \epsilon$, where ϵ is noise

- Put data into matrix vector form: (scalar y)
  - $X = \begin{pmatrix} -x_1^\top - \\ \vdots \\ -x_N^\top - \end{pmatrix} \in \mathbb{R}^{N \times n}, Y = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \in \mathbb{R}^N$
  - Minimize loss function: $l(\theta) = \|Y - X\theta\|_2^2$ (eg.$l(\theta) = \sum(y_i - \theta_0 - \theta_1 x_i)^2$)
    - Seems to make sense if noise is zero-mean

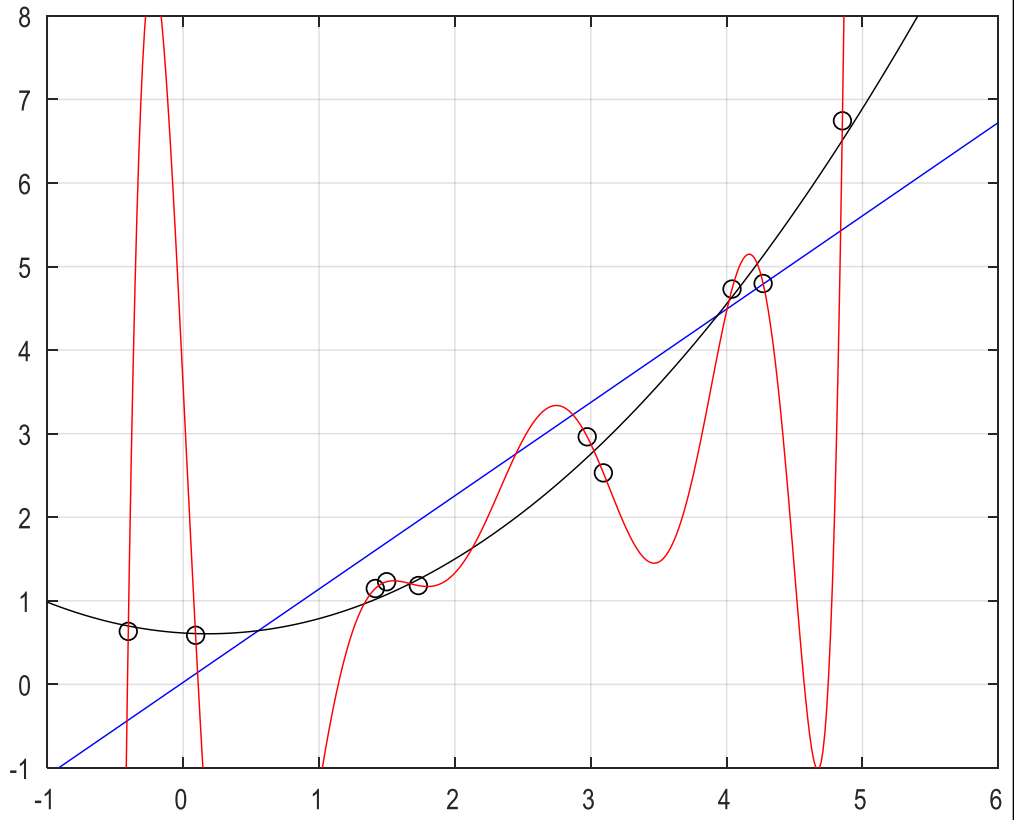
$$\theta^* = \arg\min_\theta \|Y - X\theta\|_2^2$$

$$\boldsymbol{\theta^* = \left(X^T X\right)^{-1} X^T Y}$$

Feature Augmentation

- Raw data: $\{x_i, y_i\}_{i=1}^N$
  - But perhaps $y = f(x)$ is nonlinear
  - Augment data: $\bar{x}_i = \left(1, x_i, x_i^2\right), \bar{y}_i = y_i$

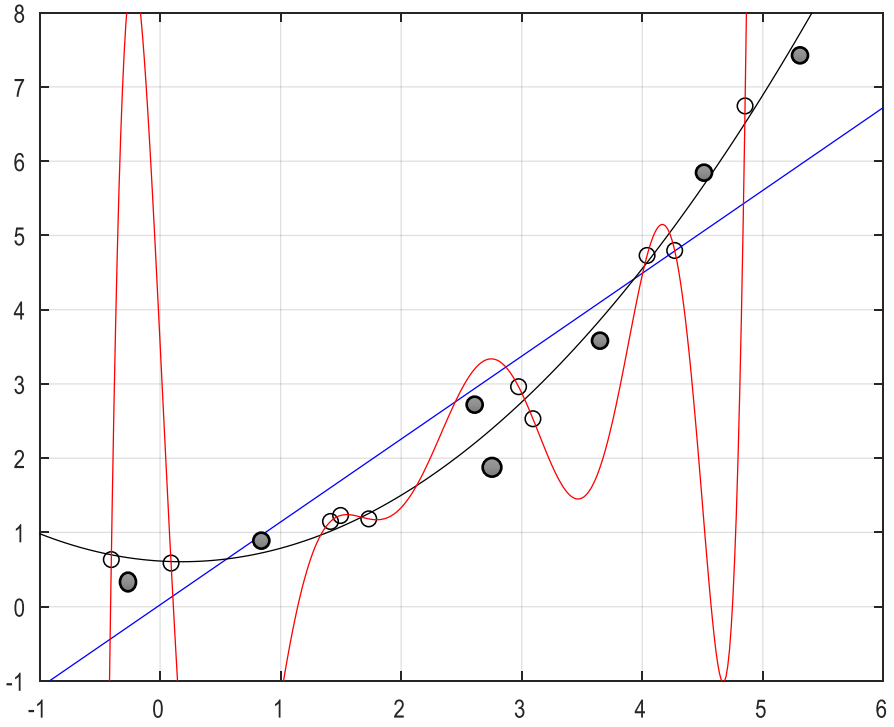
- Use linear model between $\bar{x}$ and $\bar{y}$
  - $\bar{y} = \theta^\top \bar{x} + \epsilon = \theta_0 + \theta_1 x + \theta_2 x^2 + \epsilon$
  - Effectively a quadratic model



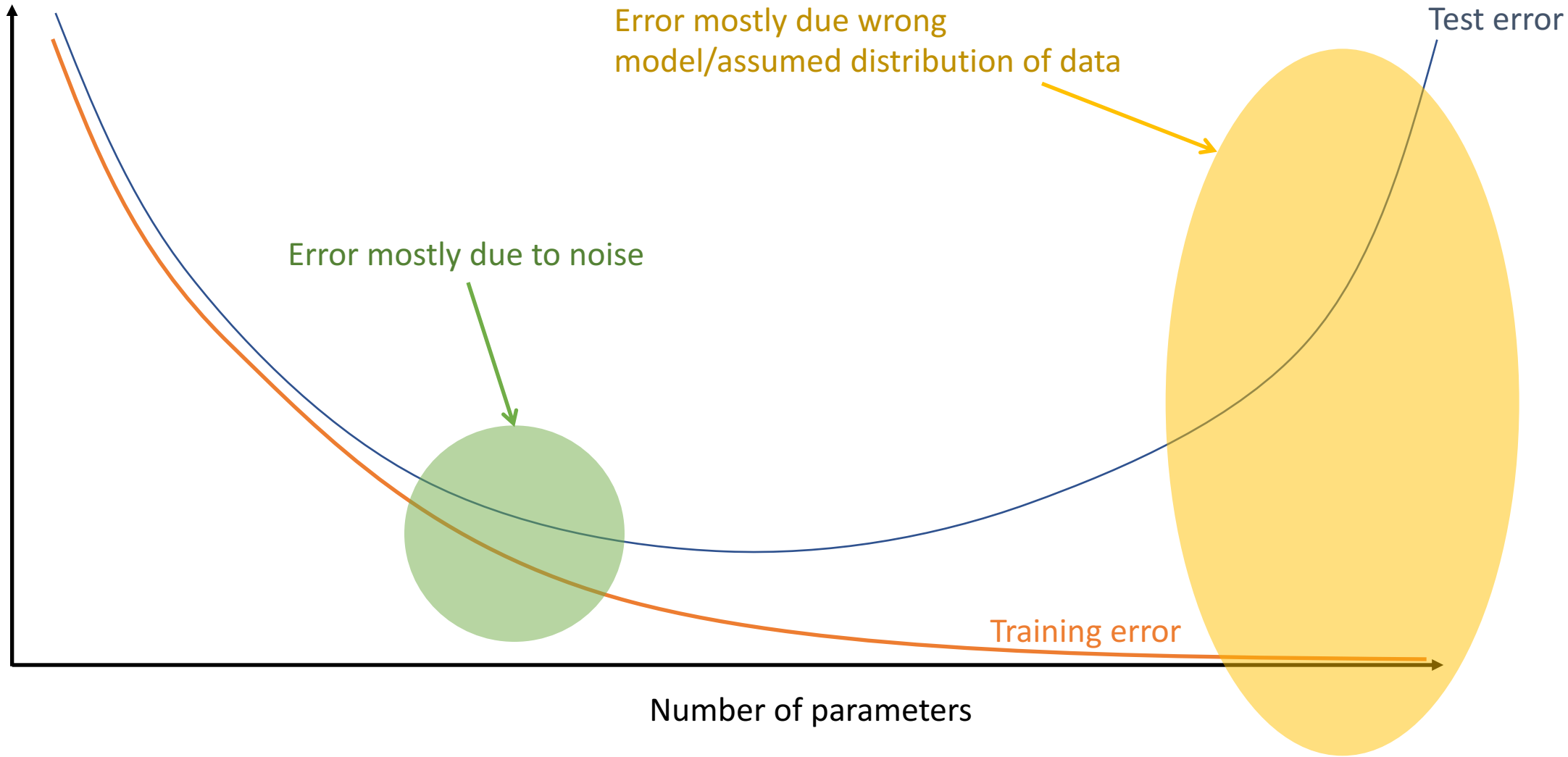
- In general, $\bar{x}_i = \left(1, x_i, x_i^2, \ldots x_i^N\right)$ → degree N polynomial
  - Correspondingly, more parameters are required

Observations

- More parameters → less training error, but potentially more test error
  - **Training error**: error when fitting model f_θ to data
  - **Test error**: error when using model to do prediction
- In our example, the true model is quadratic
  - High order polynomial would have very large test errors → overfitting
  - Assumption about distribution of data is wrong!
  - In general, the true model is unknown



Training Error and Test Error



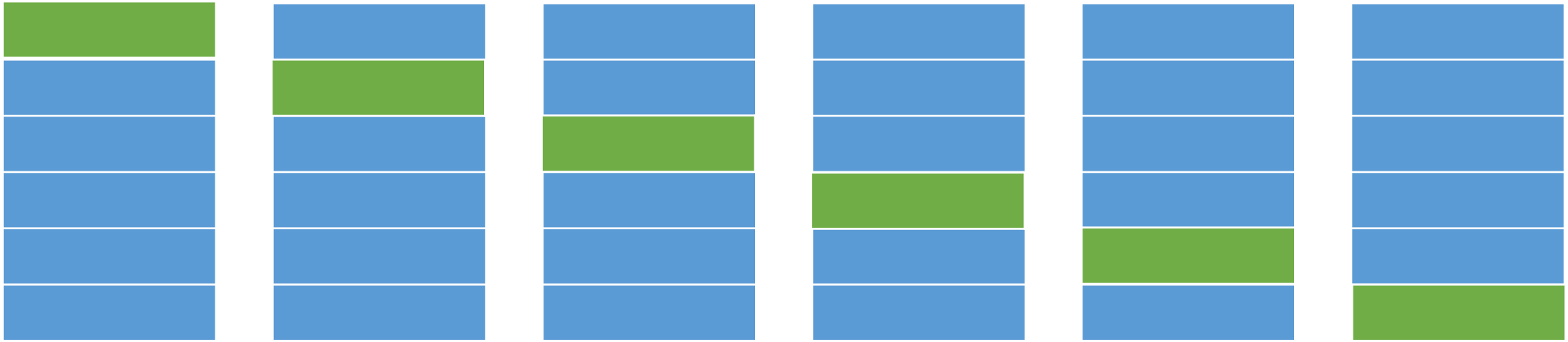
Addressing Overfitting

- Validation of Trained Models (hold-out data)
  - Divide data up into training and validation (hold-out) data
  - Do training on the training data → minimize training error
  - Validate the model on validation data → obtain **validation error**

- Regularization
  - Add penalty to size of parameters

N-Fold Cross Validation

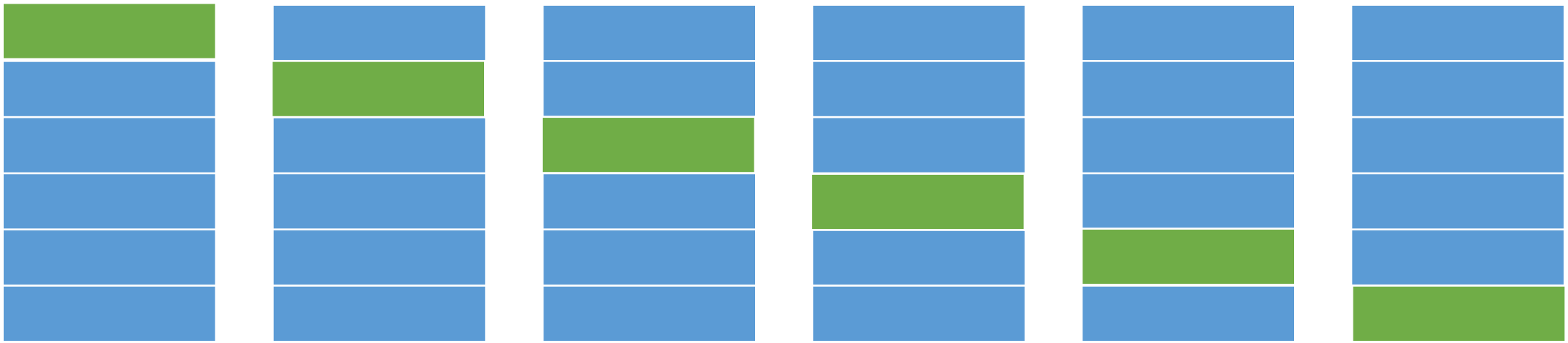
- Divide data into N (roughly) equal parts
- Go through each part
  - Do training on the other $N - 1$ parts (so one part is hold-out)
  - Evaluate model on the hold-out data to get → validation error
- Validation error is the average of all validation errors from above
  - Approximates performance during **test**, where new data is generated



N-Fold Cross Validation

- Validation error is the average of all validation errors from above
  - Approximates performance during **test**, where new data is generated

- What could still go wrong?
  - The distribution of data during test can be different from the previous data



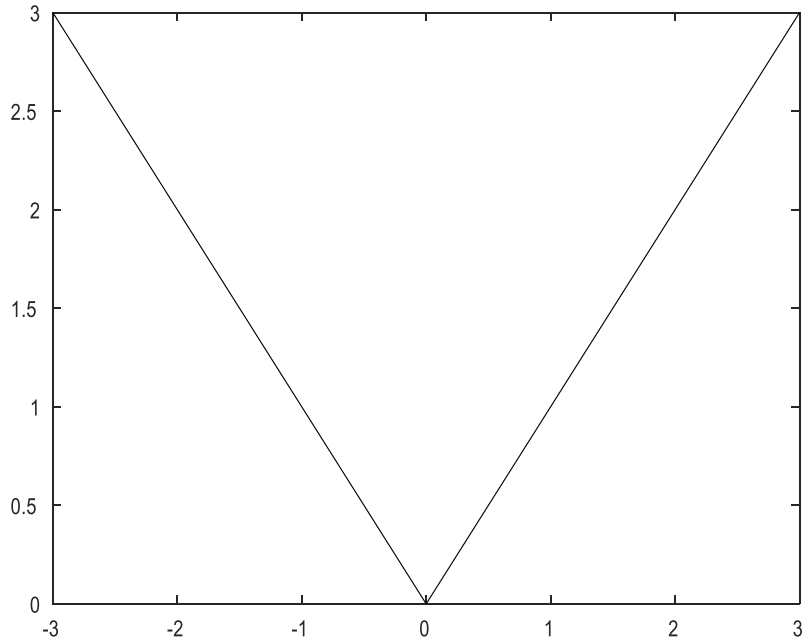
Regularization

- Previously: $l(\theta) = \|y - X\theta\|_2^2$
  - Example: $l(\theta) = \sum\left(y_i - \theta_0 - \theta_1 x_i - \theta_2 x_i^2 - \theta_3 x_i^3 - \theta_4 x_i^4\right)^2$
- L2 regularization:
  - Heuristic: the underlying ground truth model does not have large θ
  - $l(\theta) = \|Y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$
  - "**Tikhonov regularization**"
  - Statistics: "**ridge regression**"
  - Machine learning: "**weight decay**"
- L1 regularization:
  - Heuristic: many parameters in the underlying ground truth model are 0
  - $l(\theta) = \|Y - X\theta\|_2^2 + \lambda\|\theta\|_1$
  - Statistics: "**LASSO**"
  - Signal processing: "**basis pursuit**"
- "**Elastic net regularization**": combination of both
  - $l(\theta) = \|Y - X\theta\|_2^2 + \lambda\left((1-\alpha)\|\theta\|_2^2 + \alpha\|\theta\|_1\right)$

Regularization

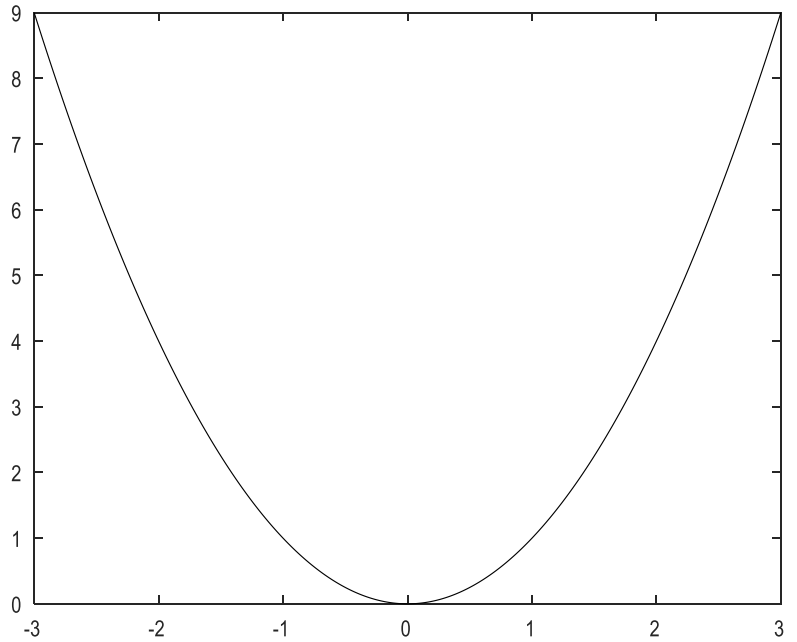
L1: $\|\boldsymbol{\theta}\|_1 = \sum_i |\boldsymbol{\theta}_i|$

- Does not prioritize reduction of any component of θ
- Encourages sparsity



L2: $\|\boldsymbol{\theta}\|_2^2 = \sum_i \boldsymbol{\theta}_i^2$

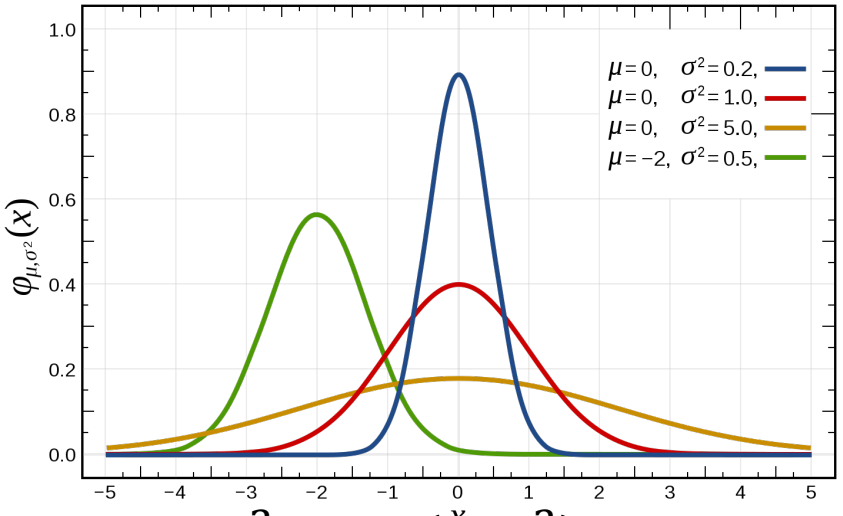
- Prioritizes reduction of large components of θ



Outline

- **Regression: two perspectives**
  - Function fitting interpretation
  - **Probabilistic interpretation**
- Classification
- Neural Networks

Maximum Likelihood Estimate



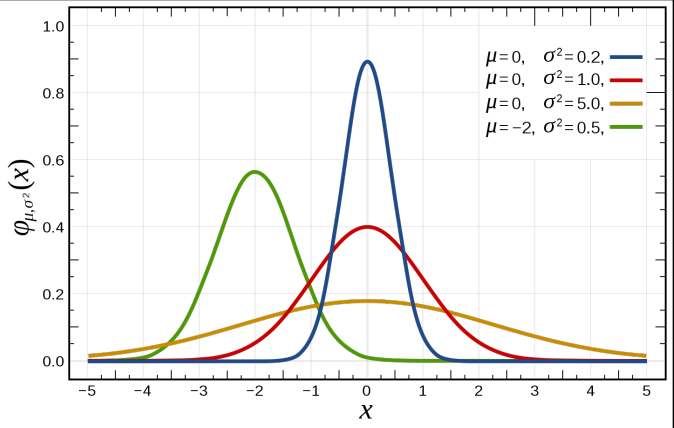
- Simplest model: Linear
  - $y = \theta^\top x + \epsilon$, where ϵ is noise
  - Assume noise is normally distributed with zero mean and variance σ^2: $\epsilon \sim N(0, \sigma^2)$
  - $y \sim N(\theta^\top x, \sigma^2)$, $p(y|\theta, x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-\theta^\top x)^2}{2\sigma^2}}$
- Data consists of $\{x_i, y_i\}_{i=1}^N$
  - Pick the θ that maximizes $p(\theta|X, Y) := p\left(\theta|\{x_i, y_i\}_{i=1}^N\right)$
  - Bayes' rule:

$$p(\theta|X, Y) = \frac{p(Y|\theta, X)p(\theta)}{p(Y)}$$

  - If we have no idea what θ should be, we can choose $p(\theta)$ to be the uniform distribution

$$\theta^* = \arg\max_\theta p(Y|\theta, X)$$

Maximum Likelihood Estimate



- Maximum likelihood estimate: $\theta^* = \arg\max_\theta p(Y|\theta, X)$
- If we assume y_i are independent and identically distributed (i.i.d.), then

$$p(Y|\theta, X) = p(y_1, y_2, \ldots, y_N|x_1, x_2, \ldots, x_N, \theta) = \prod_{i=1}^{N} p(y_i|x_i, \theta)$$

- Earlier, we assumed $y \sim N(\theta^\top x, \sigma^2)$, $p(y|\theta, x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-\theta^\top x)^2}{2\sigma^2}}$
- After some algebra, we get $\theta^* = \arg\min_\theta \|Y - X\theta\|_2^2$
  - Exactly the same result as least squares!

Maximum Likelihood Estimate: Details

$$\theta^* = \arg\max_{\theta} p(Y|\theta, X)$$

$$= \arg\max_{\theta} \prod_{i=1}^{N} p(y_i|x_i, \theta)$$

- Now, use the fact that $P_\theta(y|x) \sim N(\theta^\top x, \sigma^2)$

$$= \arg\max_{\theta} \left\{ \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - \theta^\top x_i)^2}{2\sigma^2}} \right\}$$

$$= \arg\max_{\theta} \left\{ e^{-\sum_{i=1}^{N} \frac{(y_i - \theta^\top x_i)^2}{2\sigma^2}} \right\}$$

$$= \arg\min_{\theta} \left\{ \sum_{i=1}^{N} (y_i - \theta^\top x_i)^2 \right\}$$

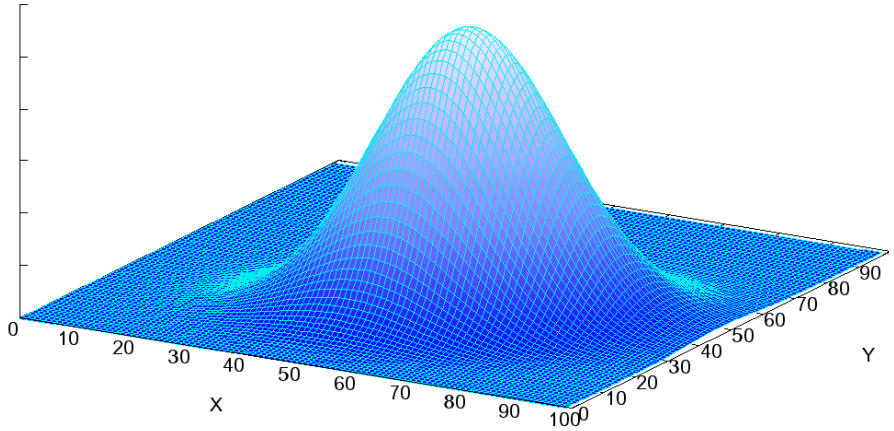
$$= \arg\min_{\theta} \|y - X\theta\|_2^2$$

Maximum A-Posteriori (MAP) Estimate

- What if we have a prior on the parameters?
  - Recall

$$p(\theta|X,Y) = \frac{p(Y|\theta,X)p(\theta)}{p(Y)}$$

  - So, we need to pick $\theta^* = \arg\max_\theta p(Y|\theta,X)p(\theta)$
  - This is the maximum a-posteriori estimate



- Suppose $\theta \sim \mathcal{N}(0, 2\lambda I)$, then after some algebra, we get

$$\theta^* = \arg\min_\theta \|Y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

  - Exactly the same as L2 regularization!

$$\boldsymbol{\theta^* = \left(X^T X + \lambda I\right)^{-1} X^T Y}$$

Maximum A-Posteriori (MAP) Estimate: Details

- We need to pick $\theta^* = \arg\max_\theta p(Y|\theta, X)p(\theta)$,
  - Suppose $\theta \sim \mathcal{N}(0, 2\lambda^{-1}I)$, then $p(\theta) = \det(4\pi\lambda^{-1}I)^{-\frac{1}{2}} e^{-\lambda\theta^\top\theta}$
- Then, we have

$$\theta^* = \arg\max_\theta p(Y|\theta, X)\, p(\theta) = \arg\max_\theta \prod_{i=1}^{N} p(y_i|x_i, \theta)\, p(\theta)$$

$$= \arg\max_\theta \left\{ \left(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - \theta^\top x_i)^2}{2\sigma^2}} \right) \det(4\pi\lambda^{-1}I)^{-\frac{1}{2}} e^{-\lambda\theta^\top\theta} \right\}$$

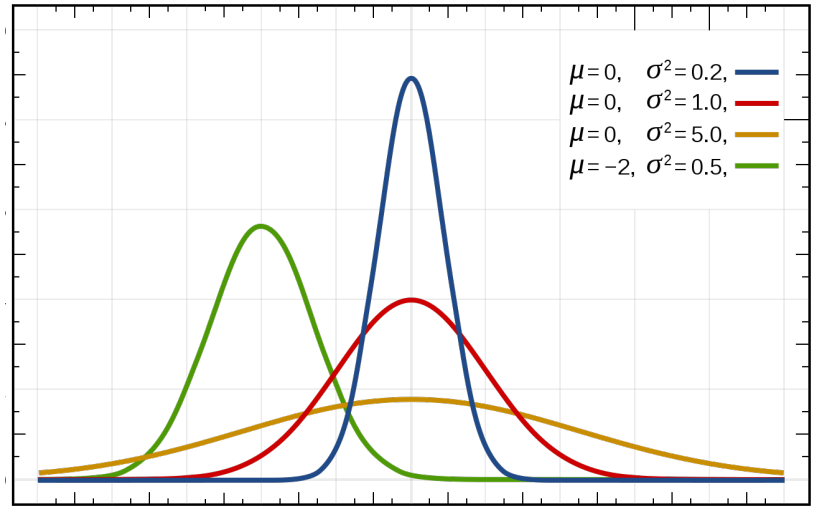
$$= \arg\max_\theta \left\{ e^{-\sum_{i=1}^{N} \frac{(y_i - \theta^\top x_i)^2}{2\sigma^2} - \lambda\theta^\top\theta} \right\}$$

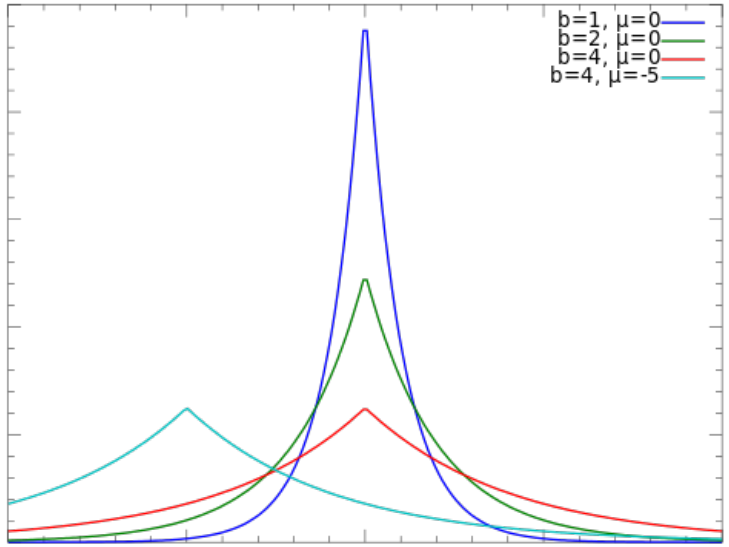
$$= \arg\min_\theta \|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

Function Fitting vs. Probabilistic Interpretation

- Assume noise is normally distributed, then the following are equivalent:
  - θ obtained from maximum likelihood
  - θ obtained from minimizing 2-norm of error
- In general, different loss functions correspond different assumptions about noise and parameter distributions
  - L2 regularization: ϵ normally distributed, θ is normally distributed
  - L1 regularization: ϵ normally distributed, θ Laplacian distributed

Normal distribution





Laplace distribution

Outline

- Regression: two perspectives
  - Function fitting interpretation
  - Probabilistic interpretation
- **Classification**
- Neural Networks

Classification

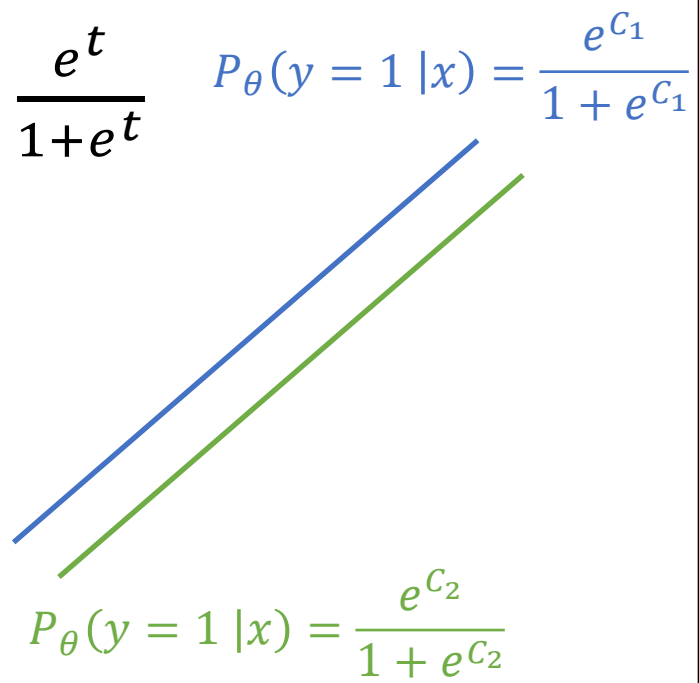
- Given $x \in \mathbb{R}^n$
  - “features”, “covariate”, “predictors”

- Predict $\boldsymbol{y \in \{0, 1\}^m}$
  - “response”, “outputs”
  - Sometimes there may be many values for each component of y
  - For example, in optical character recognition (numbers only), $y \in \{0,1, \ldots, 9\}$

- Learn the function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ such that $y \approx f(x)$
  - Use data: $\{x_i, y_i\}_{i=1}^N$

Logistic Regression

- Common model for binary classification, $y \in \{0,1\}$
- Assume $p(y = 1|x, \theta) = f\left(\sum_{i=1}^{N} \theta_i x^i\right)$ where $f(t) = \frac{e^t}{1+e^t}$
- Interpretation: Suppose $\sum_{i=1}^{N} \theta_i x^i = C$ is fixed
  - Then $p(y = 1\,|x, \theta)$ is fixed, and equal to $\frac{e^C}{1+e^C}$
    - 2D example: $\theta_1 x_1 + \theta_2 x_2 = C$ is a line
  - In addition,
    - $f(t) \to 0$ as $t \to -\infty$
    - $f(t) \to 1$ as $t \to \infty$



Logistic Regression

- Assume $p(y = 1|x, \theta) = f\left(\sum_{i=1}^{N} \theta_i x^i\right)$ where $f(t) = \frac{e^t}{1+e^t}$
  - Observe that $p(y|x, \theta) = \frac{e^{y\theta^\top x}}{1+e^{\theta^\top x}}$

- Maximize the probability by choosing θ

$$\theta^* = \arg\max_{\theta} \prod_{i=1}^{n} p(y_i|x_i, \theta)$$

Logistic Regression: Details

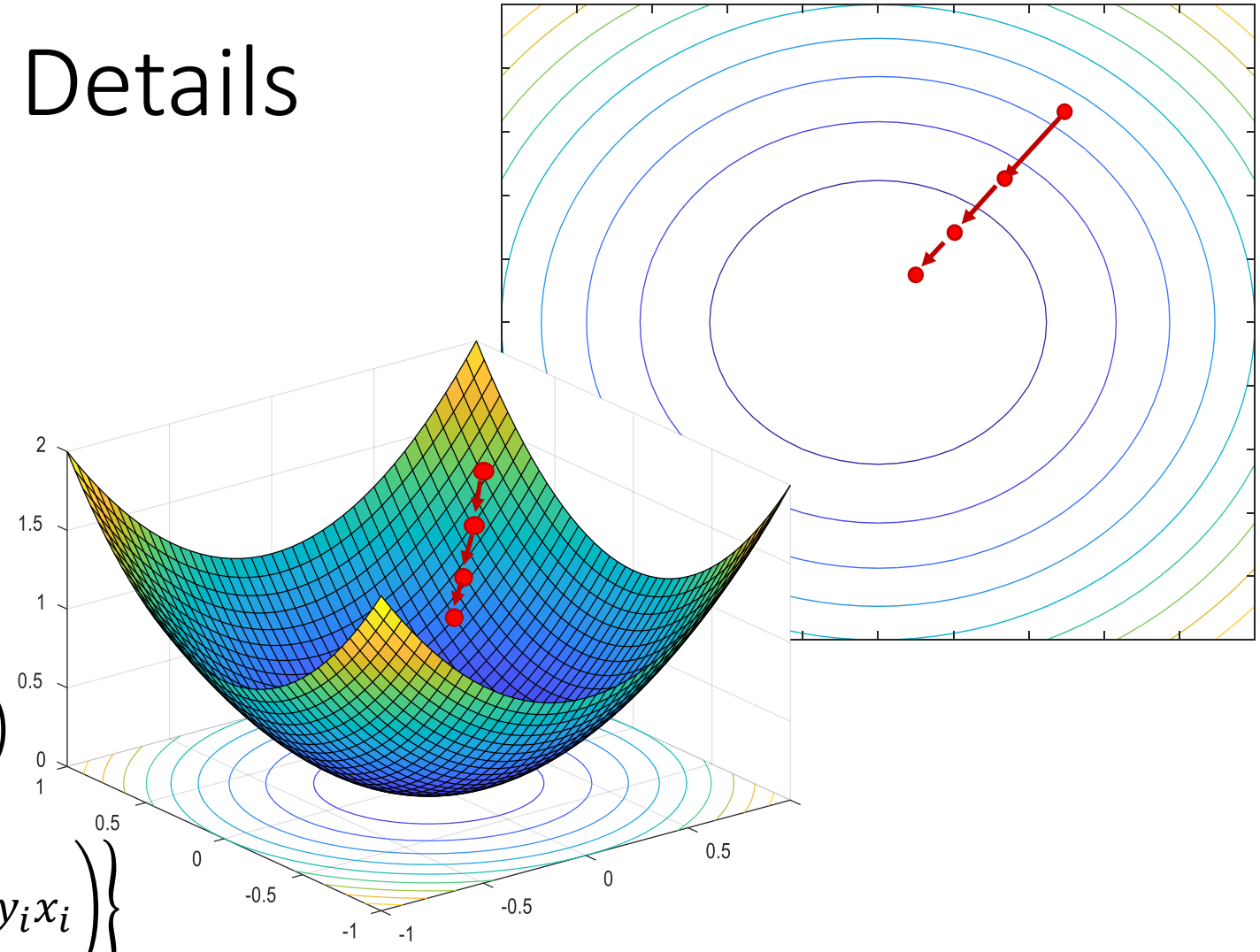
$$\theta^* = \arg\max_\theta \prod_{i=1}^{n} P_\theta(y_i|x_i)$$

$$= \arg\max_\theta \prod_{i=1}^{n} \frac{e^{y_i\theta^\top x_i}}{1+e^{\theta^\top x_i}}$$

$$= \arg\max_\theta \log\left(\prod_{i=1}^{n} \frac{e^{y_i\theta^\top x_i}}{1+e^{\theta^\top x_i}}\right)$$

$$= \arg\max_\theta \sum_{i=1}^{n} \left(y_i\theta^\top x_i - \log\left(1+e^{\bar{\theta}^T x_i}\right)\right)$$

$$= \arg\min_\theta \left\{\sum_{i=1}^{n} \underbrace{\log\left(1+e^{\theta^\top x_i}\right)} - \theta^\top\left(\sum_{i=1}^{n} y_i x_i\right)\right\}$$



$g(t) = \log(1+e^t)$ is convex → easy to solve using eg. gradient descent

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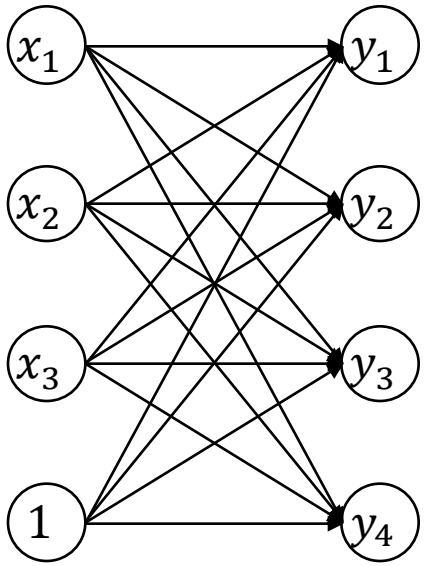
Neural Networks

- A specific form of $f_\theta(x)$



$$y_1 = f(x^\top w_1 + b_1)$$

$$y_2 = f(x^\top w_2 + b_2)$$

$$y_3 = f(x^\top w_3 + b_3)$$

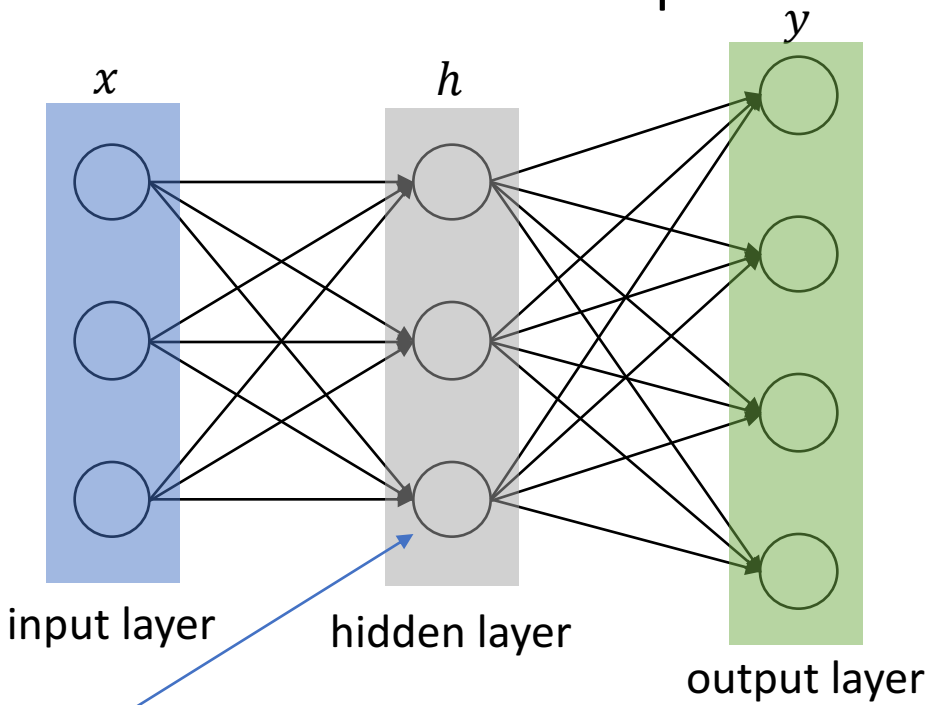
$$y_4 = f(x^\top w_4 + b_4)$$

$$y = f(x^\top W + b)$$

- Parameters θ are W and b
- "**Weights**"

Neural Networks

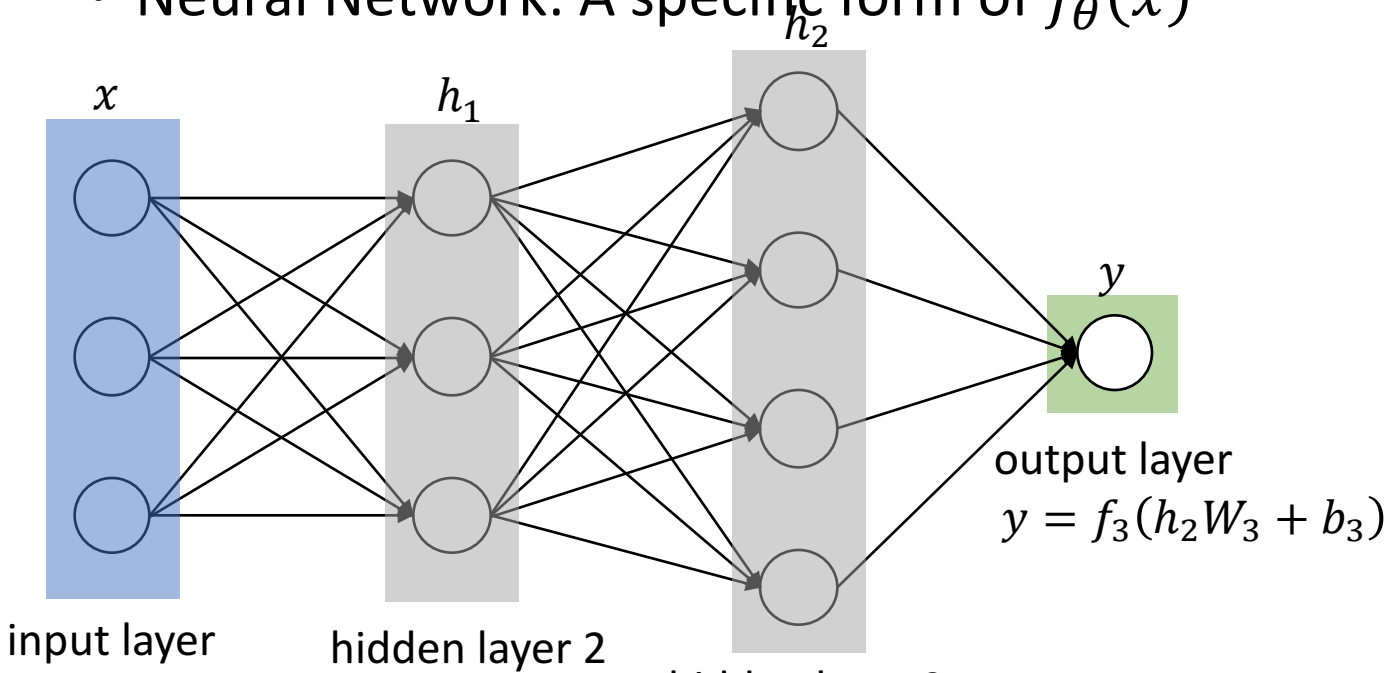
- Regression: Choose θ such that $y \approx f_\theta(x)$
  - Neural Network: A specific form of $f_\theta(x)$



$$h = f_1(x^\top W_1 + b_1) \qquad y = f_2(h^\top W_2 + b_2)$$

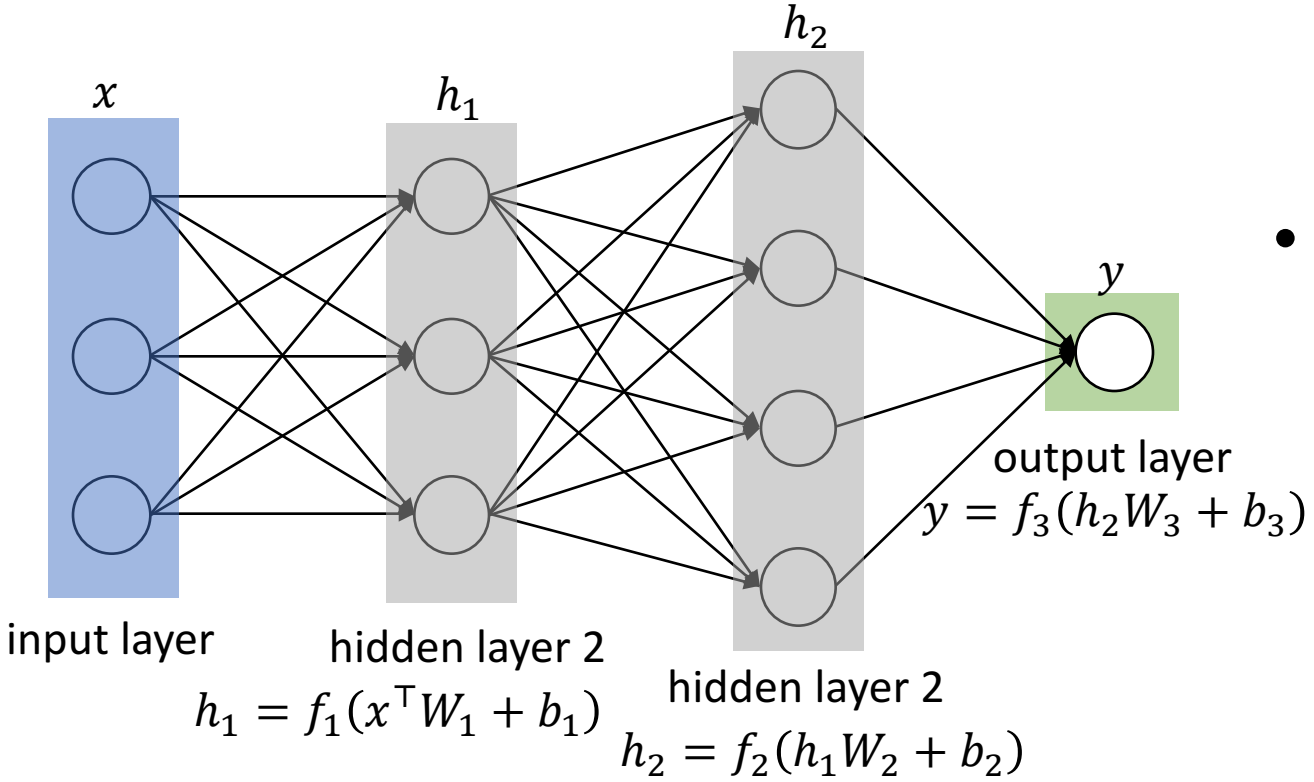
Neural Networks

- Regression: Choose θ such that $y \approx f_\theta(x)$
  - Neural Network: A specific form of $f_\theta(x)$



Neural Networks

- Regression: Choose θ such that $y \approx f_\theta(x)$
  - Neural Network: A specific form of $f_\theta(x)$



- Parameters θ are the weights W_i and b_i

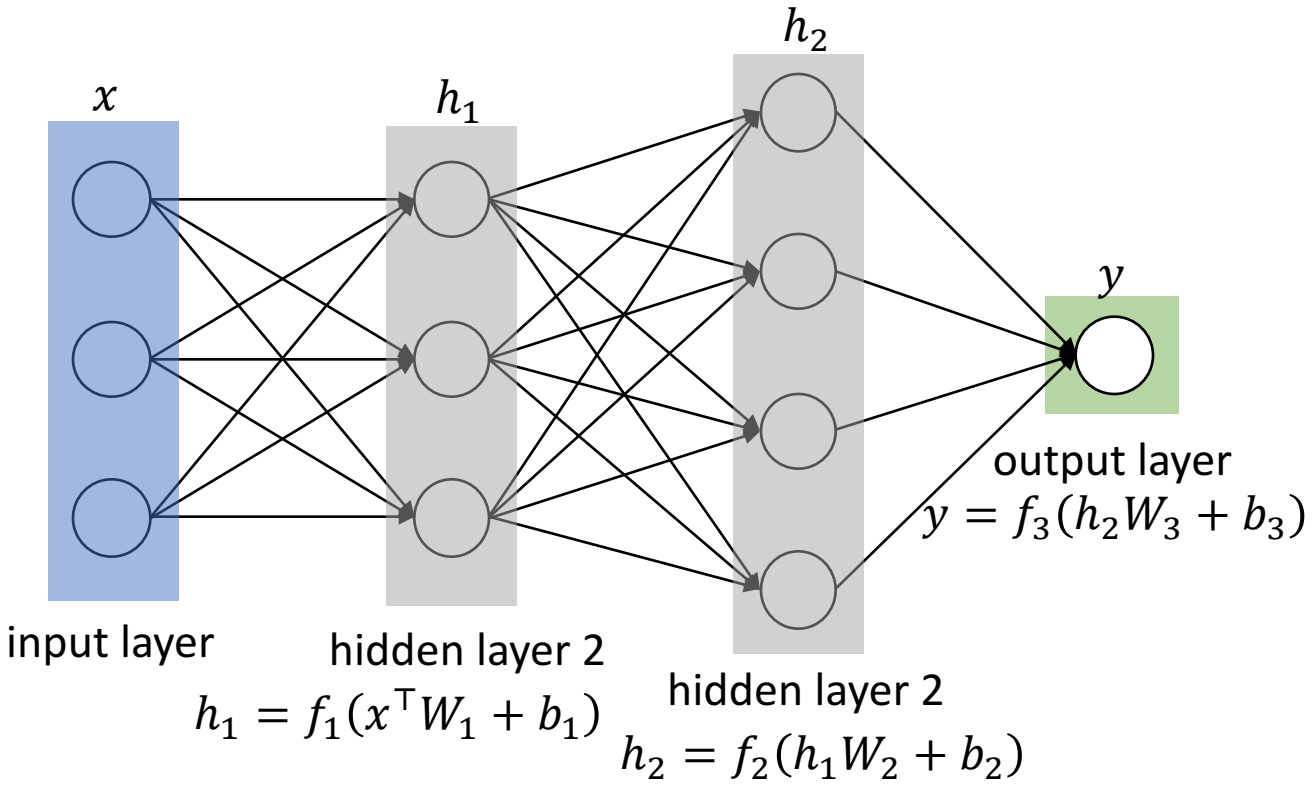
- f_1, f_2, f_3 are nonlinear
  - Otherwise f would just be a single linear function:

$$y = \big((x^\top W_1 + b_1)W_2 + b_2\big)W_3 + b_3$$
$$= x^\top W_1 W_2 W_3 + b_1 W_2 W_3 + b_2 W_3 + b_3$$

- "Activation functions"

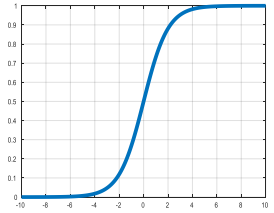
Neural Networks

- Regression: Choose θ such that $y \approx f_\theta(x)$
  - Neural Network: A specific form of $f_\theta(x)$



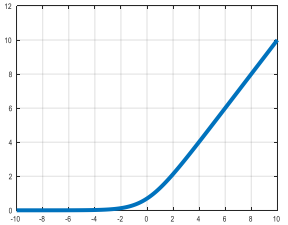
- Common choices of activation functions
  - Sigmoid:

$$\frac{1}{1 + e^{-x}}$$



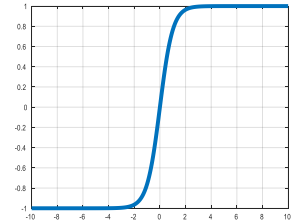
  - Softplus:

$$\log(1 + e^x)$$



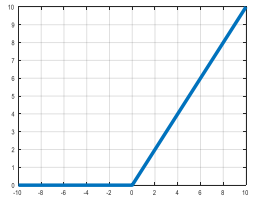
  - Hyperbolic tangent:

$$\tanh x$$



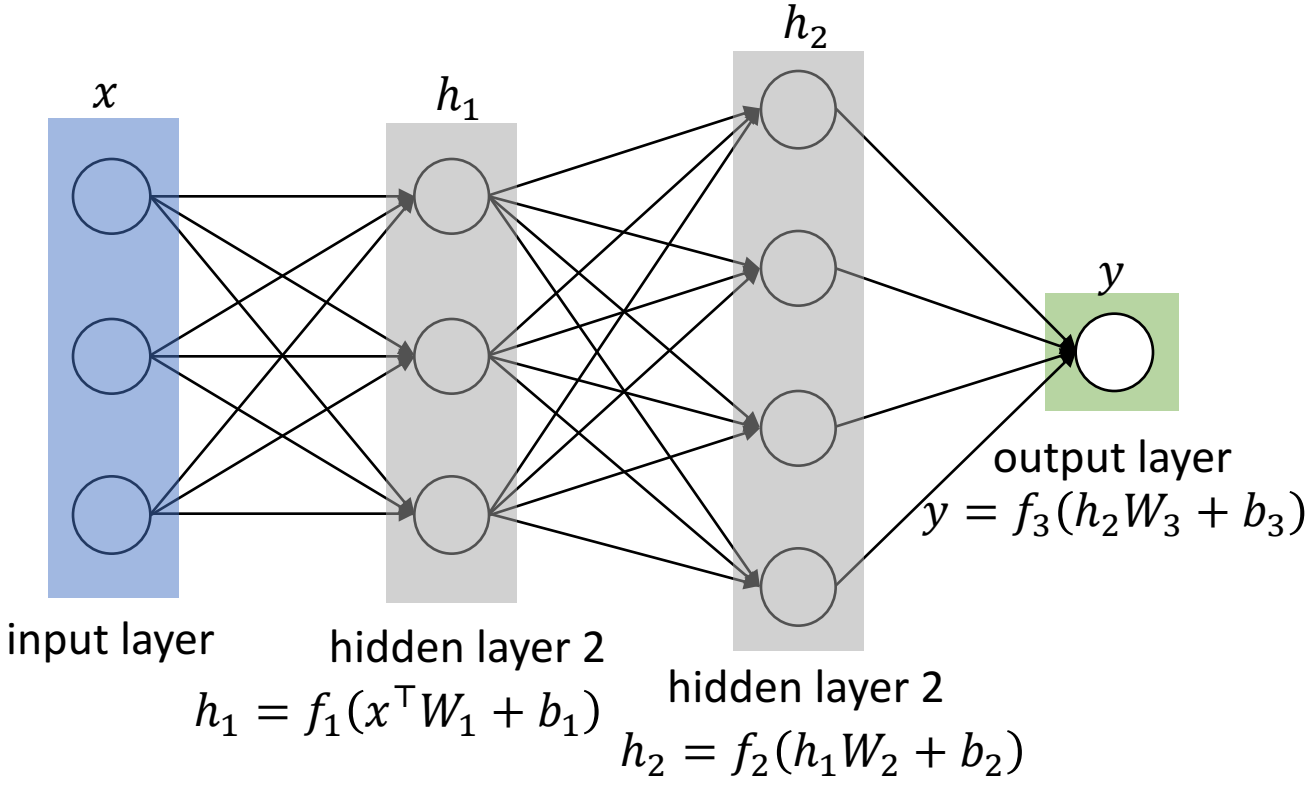
  - Rectified linear unit (ReLU):

$$\max(0, x)$$



Training Neural Networks

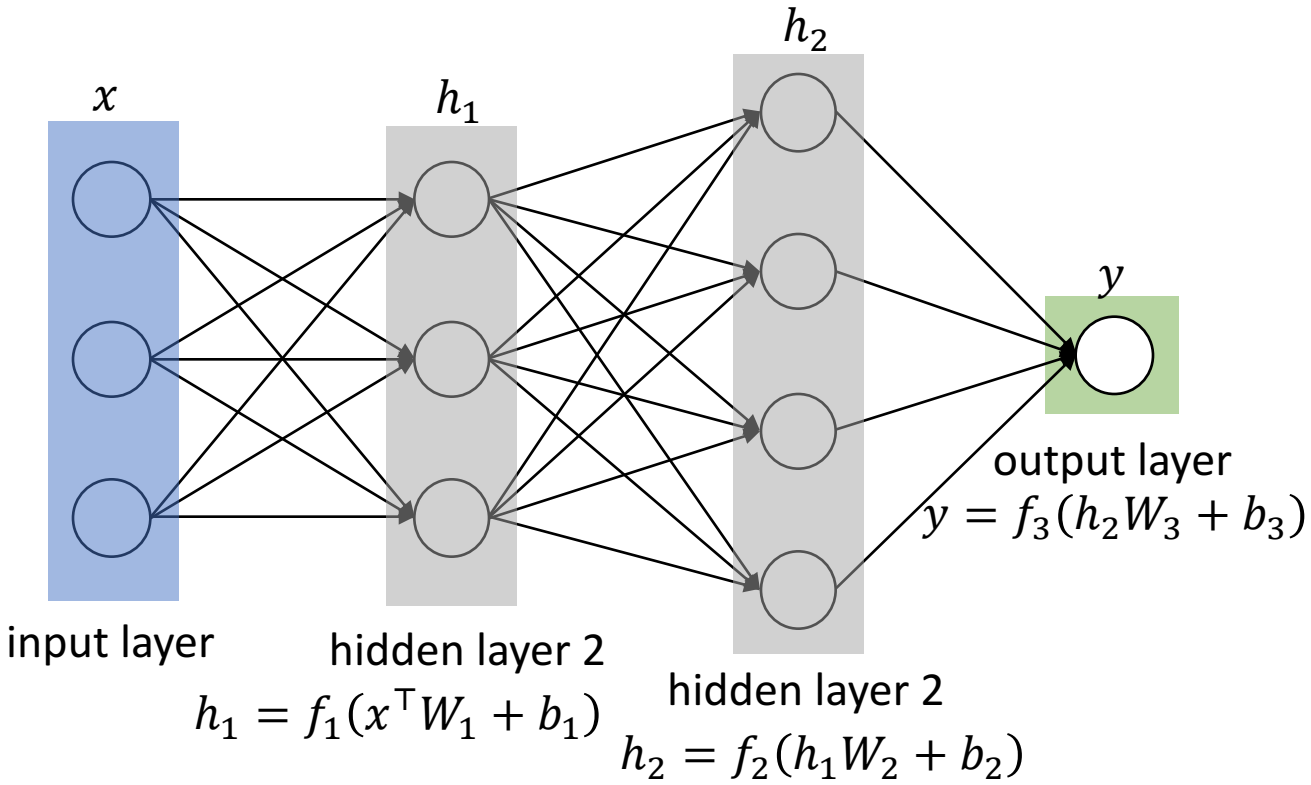
- Regression: Choose θ such that $y \approx f_\theta(x)$
  - Neural Network: A specific form of $f_\theta(x)$



- Given current θ, X, Y, compute $l(\theta; X, Y)$
  - Compares $f_\theta(X)$ with ground truth Y
  - Evaluation of f: "**Forward propagation**"

- Minimize $l(\theta; X, Y)$
  - Stochastic gradient descent
  - Evaluation of $\frac{\partial y}{\partial W}$: "**Back propagation**"
    - Example: $\frac{\partial y}{\partial W_1} = \frac{\partial y}{\partial h_2}(W_3)\frac{\partial h_2}{\partial h_1}(W_2)\frac{\partial h_1}{\partial W_1}$

Backpropagation



Example: gradient with respect to W_1

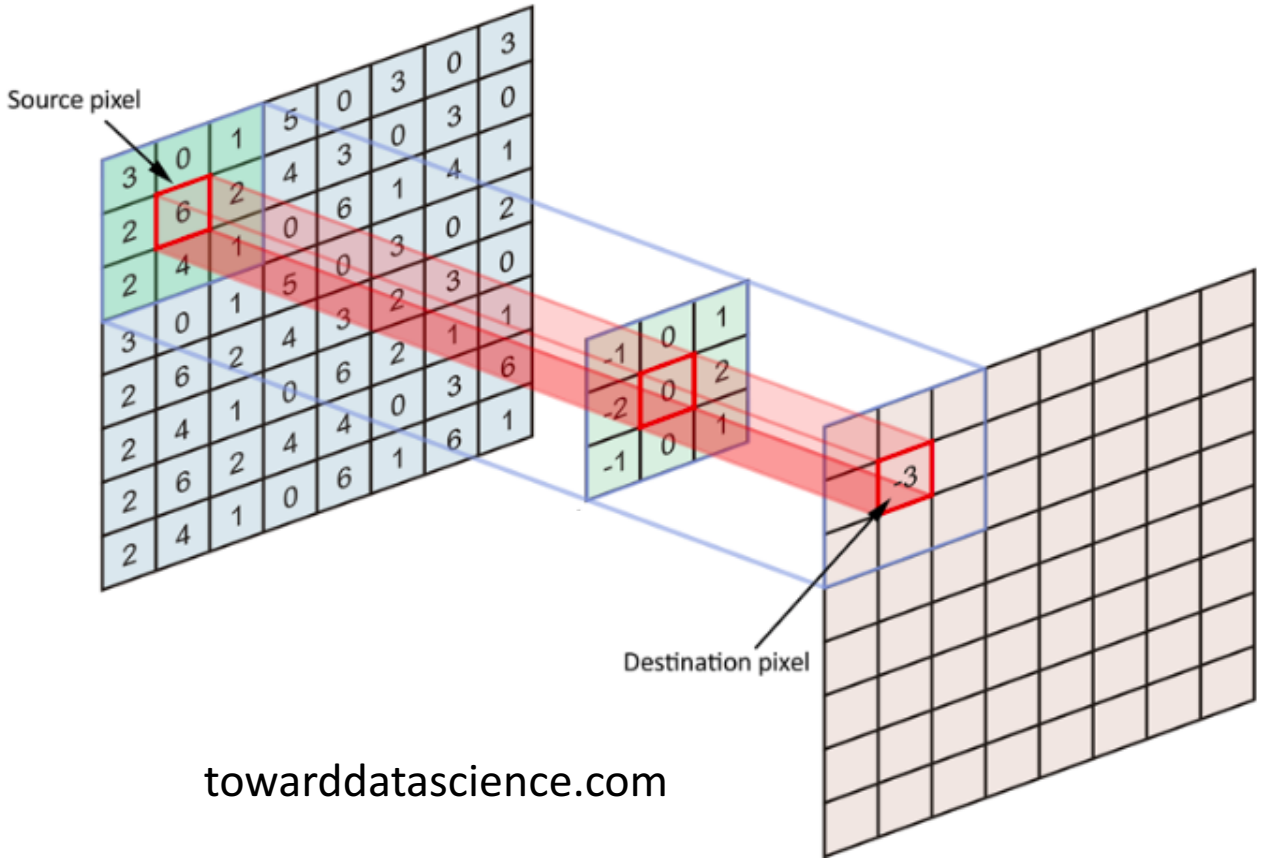
- $\frac{\partial y}{\partial W_1} = \frac{\partial f_3}{\partial h_2}\frac{\partial h_2}{\partial W_1} = \frac{\partial f_3}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial W_1}$

- Each term is a tensor, which results from taking the gradient of a vector w.r.t. a matrix

- Software like Tensorflow performs this (and other operations common in machine learning) efficiently

Common Operations

- Fully connected (dot product)
- Convolution
  - Translationally invariant
  - Controls overfitting
- Pooling (fixed function)
  - Down-sampling
  - Controls overfitting
- Nonlinearity layer (fixed function)
  - Activation functions, e.g. ReLU



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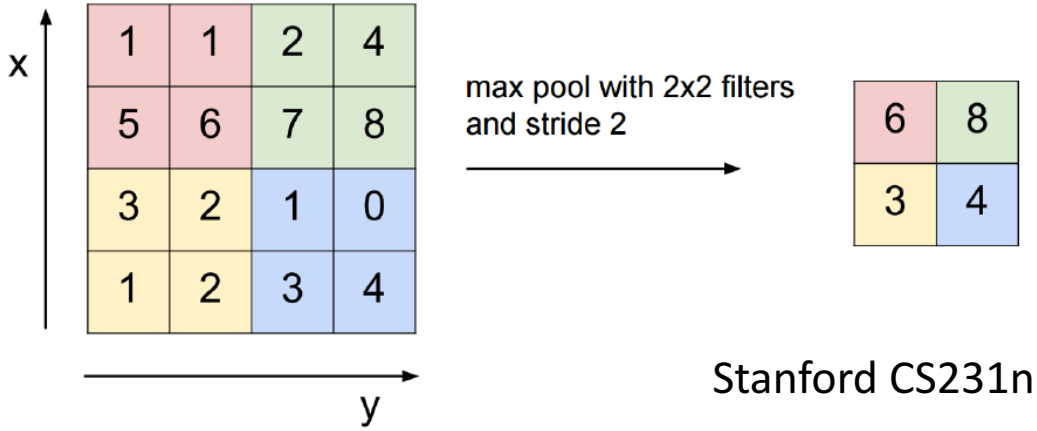
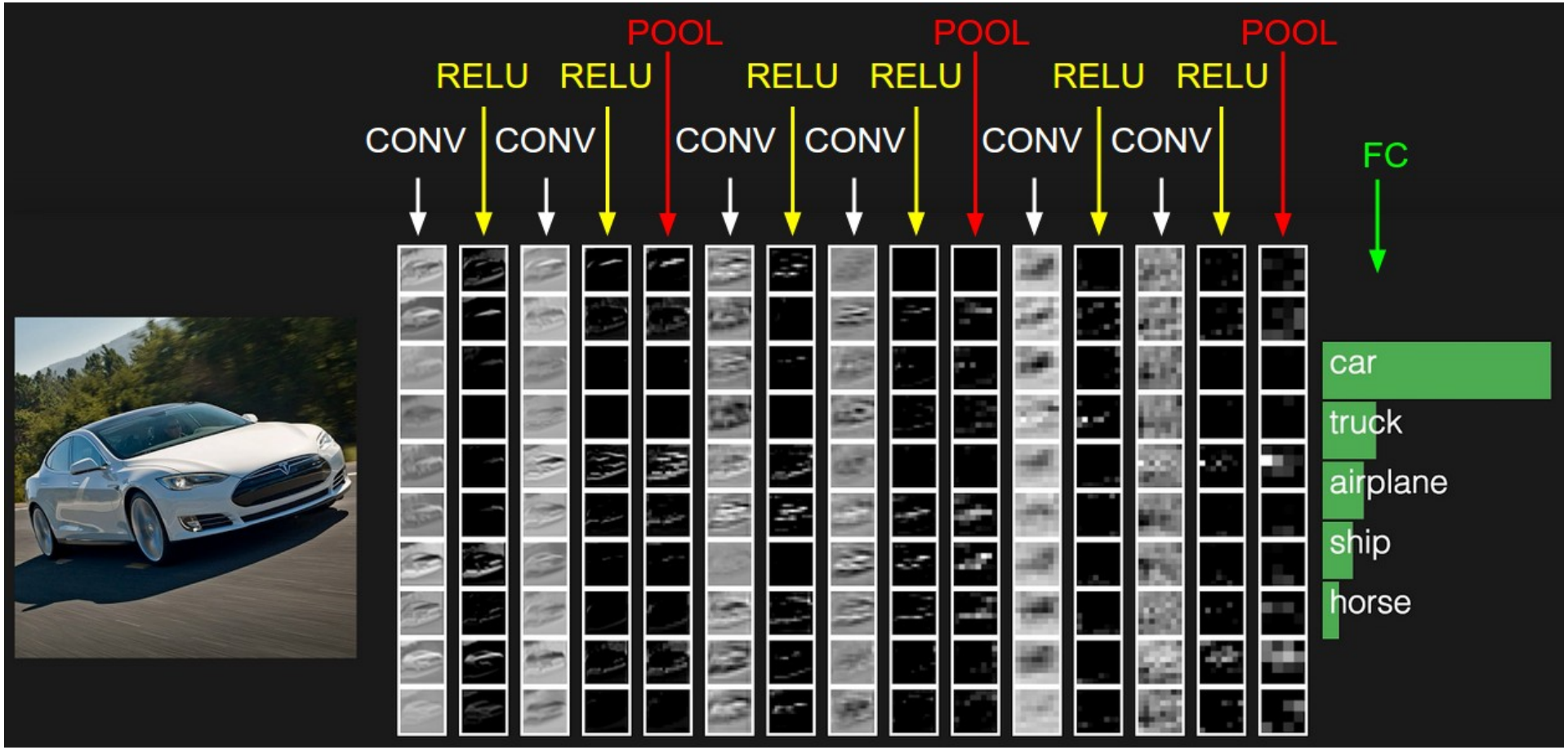


Stanford CS231n

Example: Small VGG Net From Stanford CS231n



Neural Network Architectures

- Convolutional neural network (CNN)
  - Has translational invariance properties from convolution
  - Common used for computer vision
- Recurrent neural network RNN
  - Has feedback loops to capture temporal or sequential information
  - Useful for handwriting recognition, speech recognition, reinforcement learning
  - Long short-term memory (LSTM): special type of RNN with advantages in numerical properties
- Others
  - General feedforward networks, variational autoencoders (VAEs), conditional VAEs,

Training Neural Networks

- Training process (optimization algorithm)
  - Standard L1 and L2 regularization
  - Dropout: randomly set neurons to zero in each training iteration
  - Transform input data (e.g. rotating, stretching, adding noise)
  - Learning rate (step size) and other hyperparameter tuning

- Software packages: Efficient gradient computation
  - Caffe, Torch, Theano, Tensor Flow