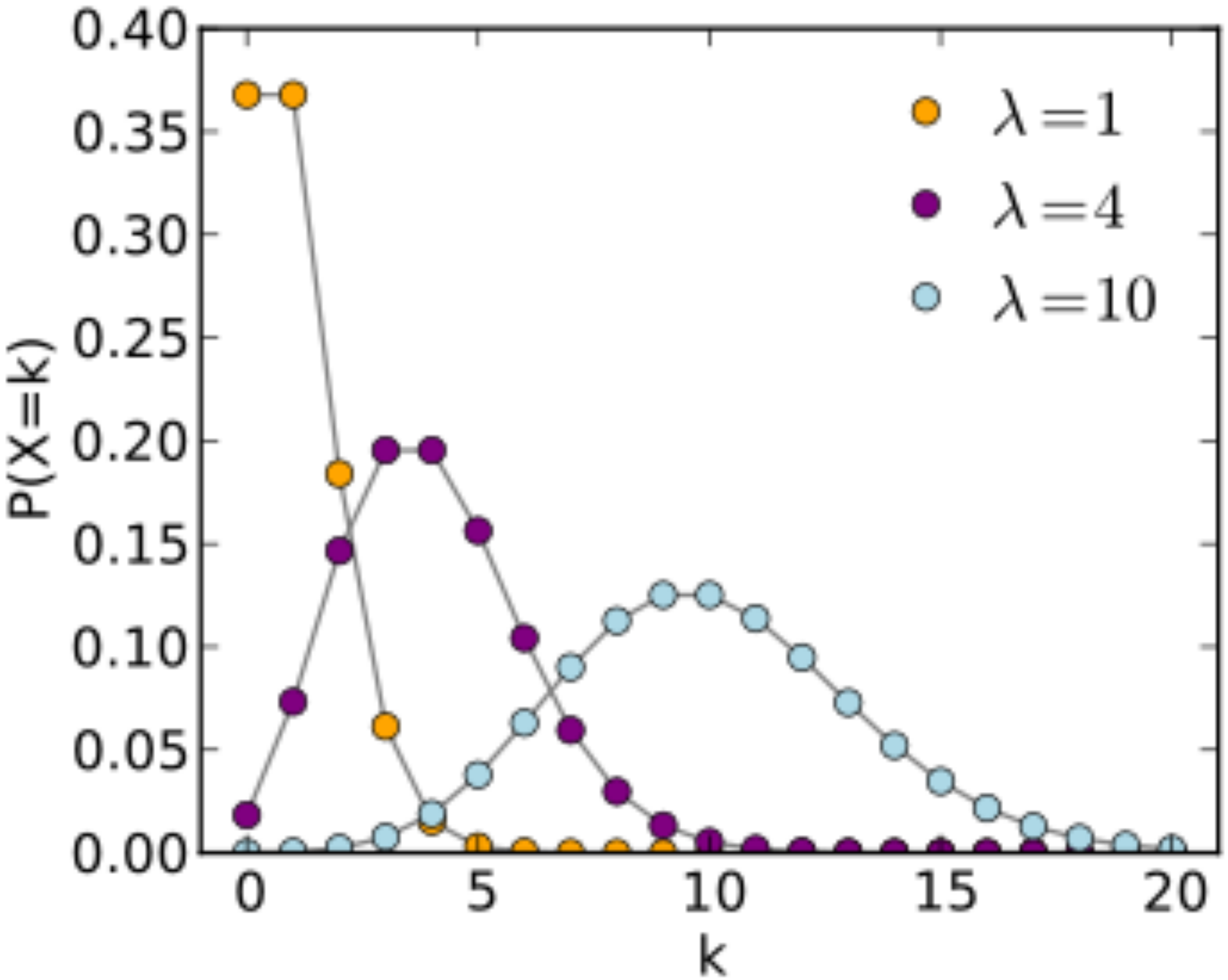
Generalized linear models and logistic regression



Comments (Oct. 15, 2019)

- Assignment 1 almost marked
  - Any questions about the problems on this assignment?
- Assignment 2 due soon
  - Any questions?

Summary so far

- From chapters 1 and 2, obtained tools needed to talk about uncertainty/noise underlying machine learning
  - capture uncertainty about data/observations using probabilities
  - formalize estimation problem for distributions
- Identify variables x_1, …, x_d
  - e.g. observed features, observed targets
- Pick the desired distribution
  - e.g. p(x_1, …, x_d) or p(x_1 | x_2, …, x_d) (conditional distribution)
  - e.g. p(x_i) is Poisson or p(y | x_1, …, x_d) is Gaussian
- Perform parameter estimation for chosen distribution
  - e.g., estimate lambda for Poisson
  - e.g. estimate mu and sigma for Gaussian

Summary so far (2)

- For prediction problems, which is much of machine learning, first discuss
  - the types of data we get (i.e., features and types of targets)
  - goal to minimize expected cost of incorrect predictions
- Concluded optimal prediction functions use p(y | x) or E[Y | x]
- From there, our goal becomes to estimate p(y|x) or E[Y | x]
- Starting from this general problem specification, it is useful to use our parameter estimation techniques to solve this problem
  - e.g., specify Y = Xw + noise, estimate mu = xw

Summary so far (3)

- For linear regression setting, modeling p(y|x) as a Gaussian with mu = <x,w> and a constant sigma
- Performed maximum likelihood to get weights w
- Possible question: why all this machinery to get to linear regression?
  - one answer: makes our assumptions about uncertainty more clear
  - another answer: it will make it easier to generalize p(y | x) to other distributions (which we will do with GLMs)

Estimation approaches for Linear regression

- Recall we estimated w for p(y I x) as a Gaussian

- We discussed the closed form solution

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

- and using batch or stochastic gradient descent

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \mathbf{X}^\top (\mathbf{X}\mathbf{w}_t - \mathbf{y})$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_t \mathbf{x}_t^\top (\mathbf{x}_t \mathbf{w}_t - y_t)$$

- **Exercise**: Now imagine you have 10 new data points. How do we get a new w, that incorporates these data points?

Exercise: MAP for Poisson

- Recall we estimated lambda for Poisson p(x)
  - Had a dataset of scalars {x1, …, xn}
  - For MLE, found the closed form solution lambda = average of xi
- Can we use gradient descent for this optimization? And if so, should we?

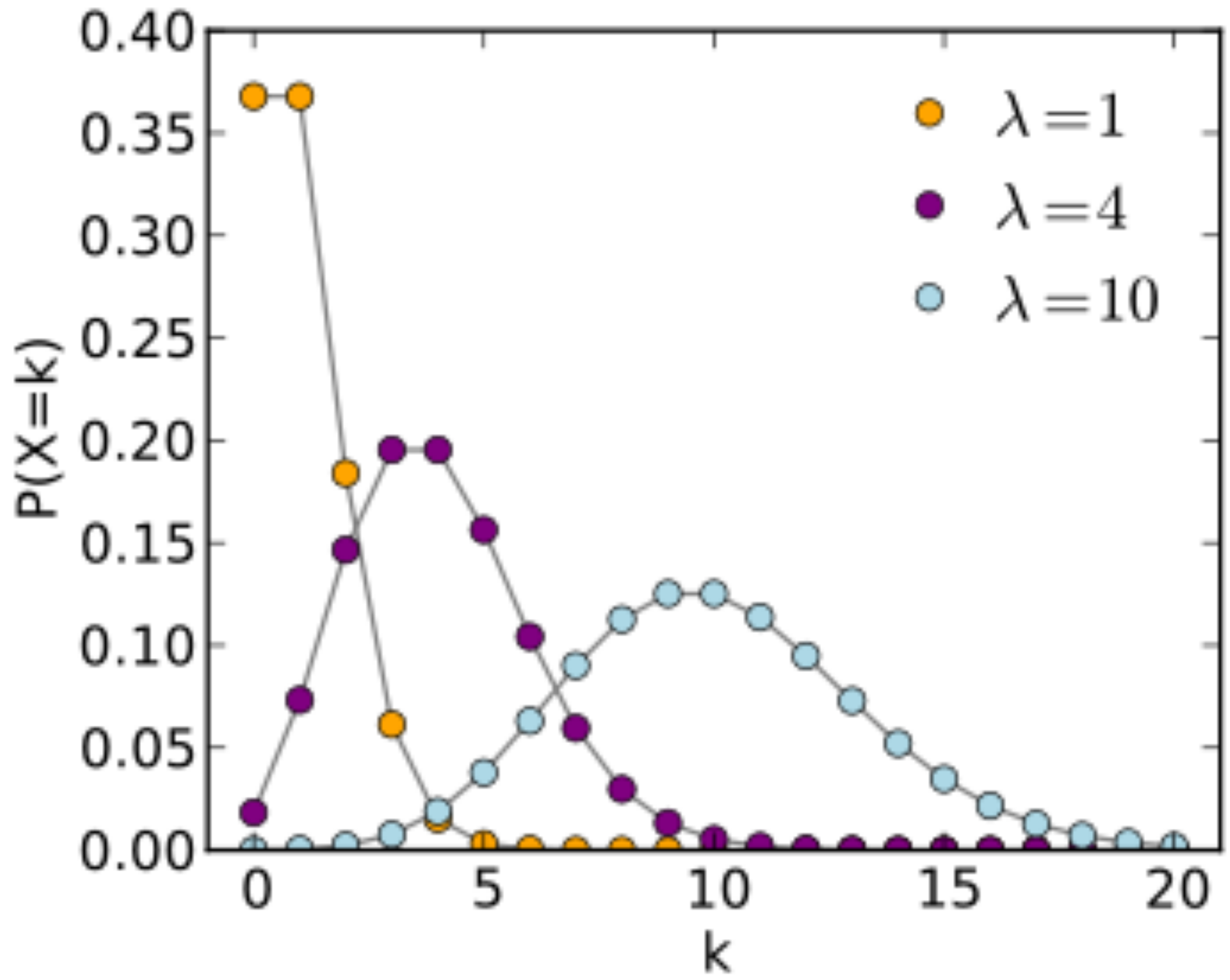
Exercise: Predicting the number of accidents

- In Assignment 1, learned p(y) as Poisson, where Y is the number of accidents in a factory
- How would the question from assignment 1 change if we also wanted to condition on features?
  - For example, want to model the number of accidents in the factory, given x1 = size of the factory and x2 = number of employees
- What is p(y | x)? What are the parameters?

Poisson regression

$$p(y|\mathbf{x}) = \text{Poisson}(y|\lambda = \exp(\mathbf{x}^\top \mathbf{w}))$$

1. $E[Y|x] = \exp(\boldsymbol{w}^\top \mathbf{x})$
2. $p(y|\mathbf{x}) = \text{Poisson}(\lambda)$



Exponential Family Distributions

$$p(y|\theta) = \exp(\theta y - a(\theta) + b(y))$$

Useful property: $$\frac{da(\theta)}{d\theta} = \mathbb{E}[Y]$$

Transfer f corresponds to the derivate of the log-normalizer function a

We will always linearly predict the natural parameter

$$\theta = \mathbf{x}^\top \mathbf{w}$$

Examples

$$\theta = \mathbf{x}^\top \mathbf{w}$$

$$p(y|\theta) = \exp(\theta y - a(\theta) + b(y))$$

- Gaussian distribution

$$a(\theta) = \frac{1}{2}\theta^2 \qquad f(\theta) = \theta$$

- Poisson distribution

$$a(\theta) = \exp(\theta) \qquad f(\theta) = \exp(\theta)$$

- Bernoulli distribution

$$a(\theta) = \ln(1 + \exp(\theta)) \qquad f(\theta) = \frac{1}{1 + \exp(-\theta)}$$

sigmoid

Exercise: How do we extract the form for the Poisson distribution?

$$p(y|\theta) = \exp(\theta y - a(\theta) + b(y))$$

Example 17: The Poisson distribution can be expressed as

$$p(x|\lambda) = \exp\left(x \log \lambda - \lambda - \log x!\right),$$

where $\lambda \in \mathbb{R}^+$ and $\mathcal{X} = \mathbb{N}_0$. Thus, $\theta = \log \lambda$, $a(\theta) = e^\theta$, and $b(x) = -\log x!$.

- What is the transfer f?

$$f(\theta) = \frac{da(\theta)}{d\theta} = \exp(\theta)$$

Exercise: How do we extract the form for the exponential distribution?

$$\lambda > 0 \qquad \lambda \exp(-\lambda y)$$

- Recall exponential family distribution

$$p(y|\theta) = \exp(\theta y - a(\theta) + b(y))$$

i.e., $p(y|\theta) = \exp(\theta y) \exp(-a(\theta)) \exp(b(y))$

- How do we write the exponential distribution this way?

$$\theta = \mathbf{x}^\top \mathbf{w} \qquad a(\theta) = -\ln(-\theta) \qquad b(y) = 0$$

- What is the transfer f?

$$f(\theta) = \frac{d}{d\theta} a(\theta) = \frac{-1}{\theta}$$

Logistic regression

$$\alpha = p(y = 1|\mathbf{x})$$

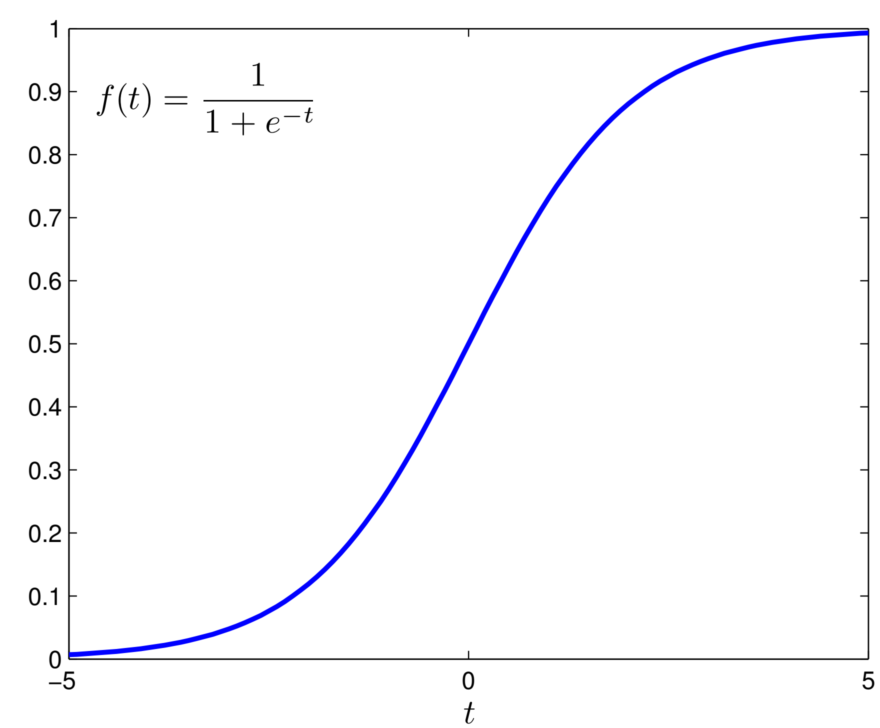
1. $E[y|\mathbf{x}] = \sigma(\boldsymbol{\omega}^\top \mathbf{x})$
2. $p(y|\mathbf{x}) = \text{Bernoulli}(\alpha)$ with $\alpha = E[y|\mathbf{x}]$.

The Bernoulli distribution, with α a function of $\mathbf{x}$, is

$$p(y|\mathbf{x}) = \begin{cases} \left(\frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right)^y & \text{for } y = 1 \\ \left(1 - \frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right)^{1-y} & \text{for } y = 0 \end{cases}$$
$$= \sigma(\mathbf{x}^\top \mathbf{w})^y (1 - \sigma(\mathbf{x}^\top \mathbf{w}))^{1-y}$$

$$E[y|\mathbf{x}] = \frac{1}{1 + e^{-\boldsymbol{\omega}^T \mathbf{x}}}$$

$$p(y|\mathbf{x}) = \left(\frac{1}{1 + e^{-\omega^T \mathbf{x}}}\right)^y \left(1 - \frac{1}{1 + e^{-\omega^T \mathbf{x}}}\right)^{1-y}.$$



What is c(w) for GLMs?

- Still formulating an optimization problem to predict targets y given features **x**
- The variables we learn is the weight vector **w**
- What is c(**w**)? $MLE: c(\mathbf{w}) \propto -\ln p(\mathcal{D}|\mathbf{w})$

$$\propto -\sum_{i=1}^{n} \ln p(y_i|\mathbf{x}_i\mathbf{w})$$

- $$\arg\min_{\mathbf{w}} c(\mathbf{w}) = \arg\max_{\mathbf{w}} p(\mathcal{D}|\mathbf{w})$$

Cross-entropy loss for Logistic Regression

$$c_i(\mathbf{w}) = y_i \ln \sigma(\mathbf{w}^\top \mathbf{x}_i) + (1 - y_i) \ln(1 - \sigma(\mathbf{w}^\top \mathbf{x}_i))$$

Extra exercises

- Go through the derivation of $c(w)$ for logistic regression
- Derive Maximum Likelihood objective in Section 8.1.2

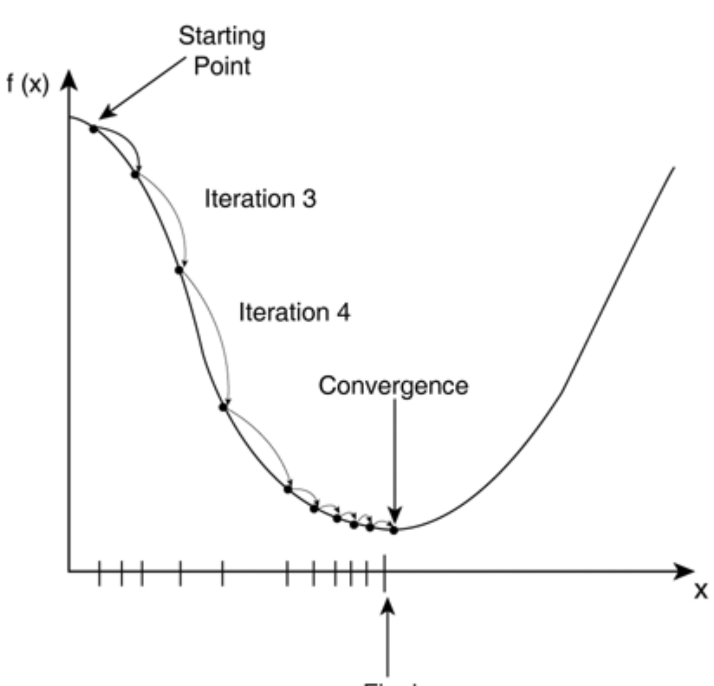
Benefits of GLMs

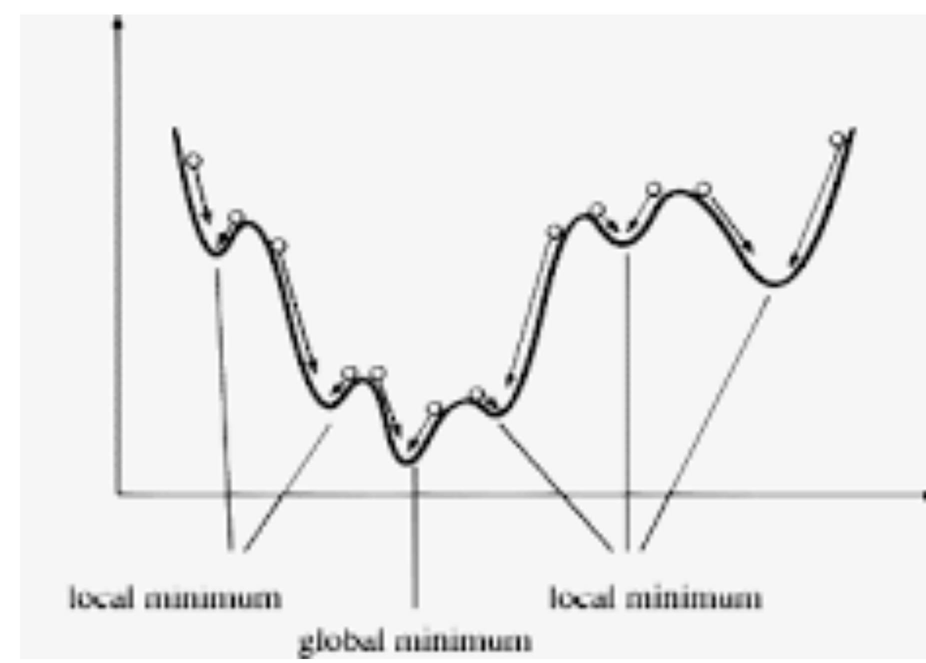
- Gave a generic update rule, where you only needed to know the transfer for your chosen distribution
  - e.g., linear regression with transfer f = identity
  - e.g., Poisson regression with transfer f = exp
  - e.g., logistic regression with transfer f = sigmoid
- We know the objective is convex in w!

Convexity

- Convexity of negative log likelihood of (many) exponential families
  - The negative log likelihood of many exponential families is convex, which is an important advantage of the maximum likelihood approach

- Why is convexity important?
  - e.g.,(sigmoid(xw) - y)^2 is nonconvex, but who cares?





Cross-entropy loss versus Euclidean loss for classification

$$c_i(\mathbf{w}) = y_i \ln \sigma(\mathbf{w}^\top \mathbf{x}_i) + (1 - y_i) \ln(1 - \sigma(\mathbf{w}^\top \mathbf{x}_i))$$

- Why not just use

$$\min_{\mathbf{w} \in \mathbb{R}^d} \sum_{i=1}^{n} (\sigma(\mathbf{x}_i^\top \mathbf{w}) - y_i)^2$$

- The notes explain that this is a non-convex objective
  - from personal experience, it seems to do more poorly in practice
- If no obvious reason to prefer one or the other, we may as well pick the objective that is convex (no local minima)

How can we check convexity?

- Can check the definition of convexity

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

- Can check second derivative for scalar parameters (e.g. λ) and Hessian for multidimensional parameters (e.g., $\mathbf{w}$)
  - e.g., for linear regression (least-squares), the Hessian is $\mathbf{H} = \mathbf{X}^\top \mathbf{X}$ and so positive semi-definite
  - e.g., for Poisson regression, the Hessian of the negative log-likelihood is $\mathbf{H} = \mathbf{X}^\top \mathbf{C} \mathbf{X}$ and so positive semi-definite

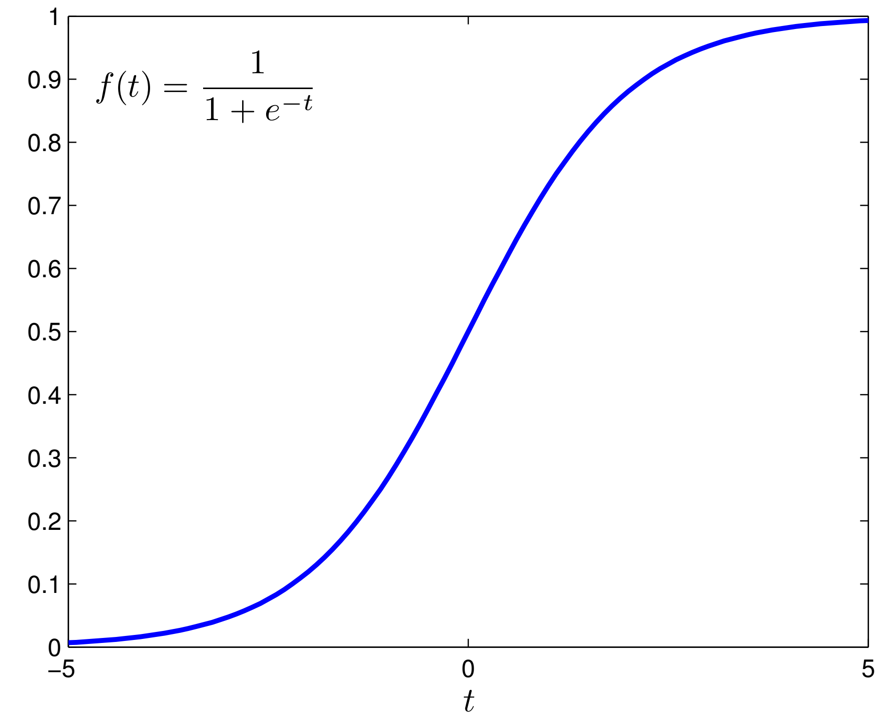
Prediction with logistic regression

- So far, we have used the prediction f(xw)
  - eg., xw for linear regression, exp(xw) for Poisson regression

- For binary classification, want to output 0 or 1, rather than the probability value p(y = 1 | x) = sigmoid(xw)

- Sigmoid has few values xw mapped close to 0.5; most values somewhat larger than 0 are mapped close to 0 (and vice versa for 1)

- Decision threshold:
  - sigmoid(xw) < 0.5 is class 0
  - sigmoid(xw) > 0.5 is class 1



Logistic regression is a linear classifier

- Hyperplane $\mathbf{w}^\top \mathbf{x} = 0$ separates the two classes
  - P(y=1 | x, w) > 0.5 only when $\mathbf{w}^\top \mathbf{x} \geq 0.$
  - P(y=0 | x, w) > 0.5 only when P(y=1 | x, w) < 0.5, which happens when $\mathbf{w}^\top \mathbf{x} < 0$

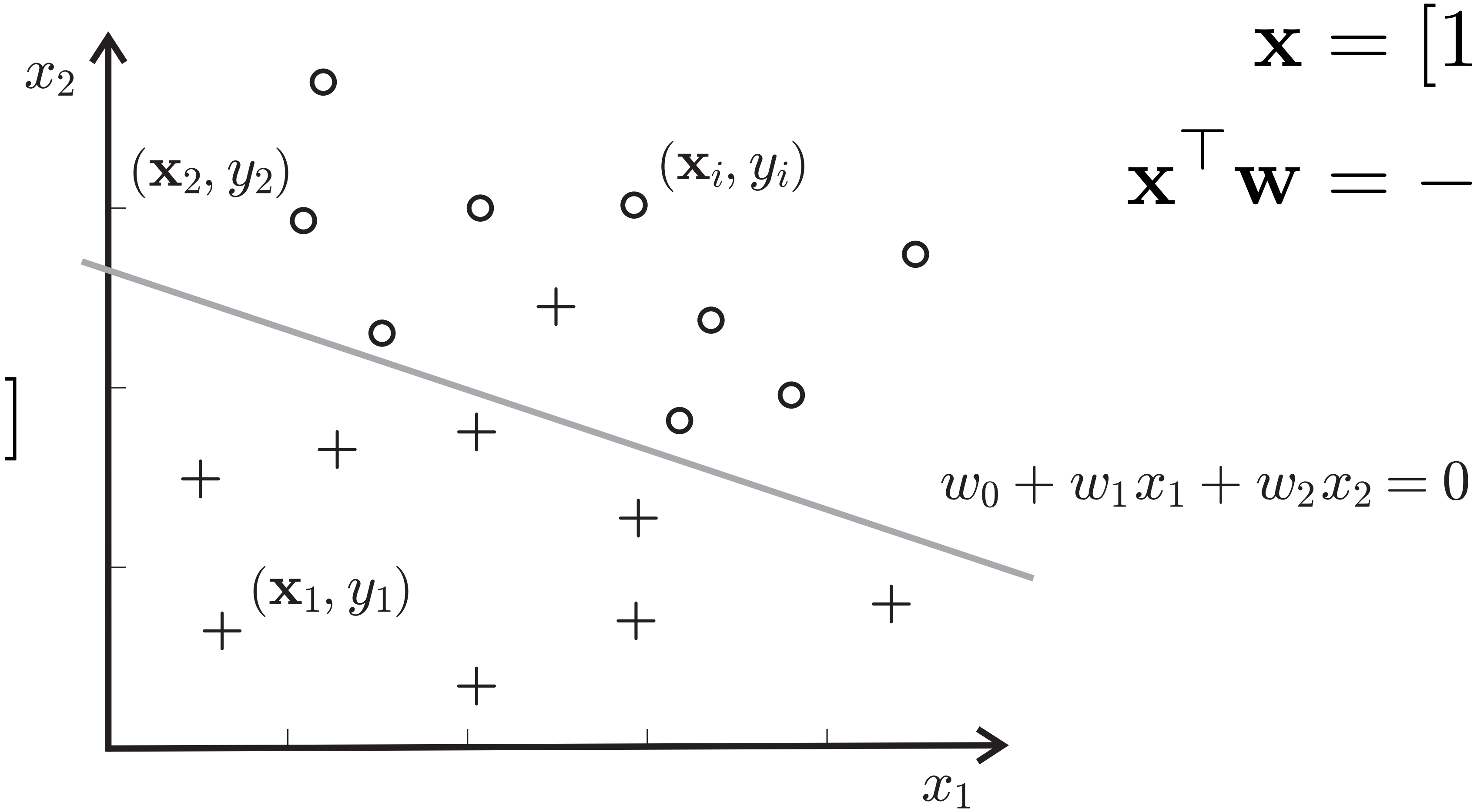
$$\text{e.g., } \mathbf{w} = [2.75 \;\; \text{-}1/3 \;\; \text{-}1]$$

$$\mathbf{x} = [1 \;\; 4 \;\; 3]$$

$$\mathbf{x}^\top \mathbf{w} = -1.8$$

$$\mathbf{x} = [1 \;\; 2 \;\; 1]$$

$$\mathbf{x}^\top \mathbf{w} = 0.27$$



Logistic regression versus Linear regression

- Why might one be better than the other? They both use a linear approach

- Linear regression could still learn <x, w> to predict E[Y | x]

- Demo: logistic regression performs better under outliers, when the outlier is still on the correct side of the line

- Conclusion:
  - logistic regression better reflects the goals of predicting p(y=1 | x), to finding separating hyperplane
  - Linear regression assumes E[Y | x] a linear function of x!

Adding regularizers to GLMs

- How do we add regularization to logistic regression?
- We had an optimization for logistic regression to get w: minimize negative log-likelihood, i.e. minimize cross-entropy
- Now want to balance negative log-likelihood and regularizer (i.e., the prior for MAP)
- Simply add regularizer to the objective function

Adding a regularizer to logistic regression

- Original objective function for logistic regression

$$\arg\max_{\mathbf{w}} \sum_{i=1}^{n} \left((y_i - 1)\, \mathbf{w}^\top \mathbf{x}_i + \log \left(\frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \right)$$

$$\arg\min_{\mathbf{w}} - \sum_{i=1}^{n} \left((y_i - 1)\, \mathbf{w}^\top \mathbf{x}_i + \log \left(\frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \right)$$

- Adding regularizer

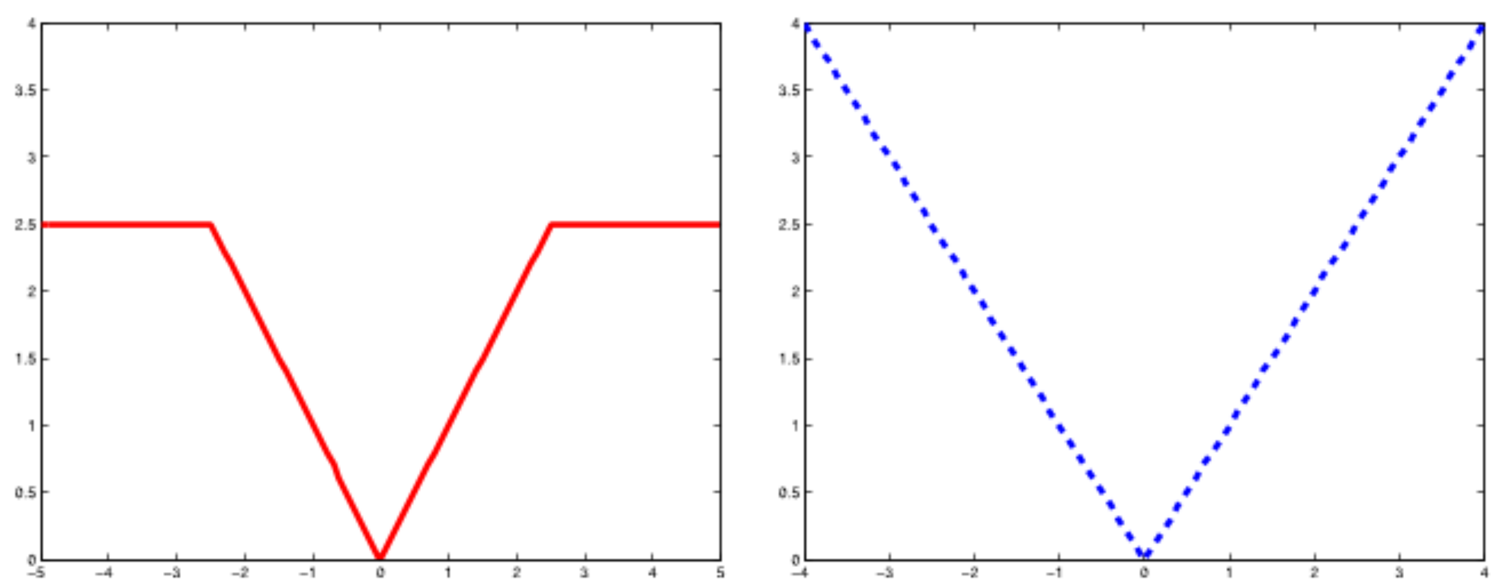
$$\arg\min_{\mathbf{w}} - \sum_{i=1}^{n} \left((y_i - 1)\, \mathbf{w}^\top \mathbf{x}_i + \log \left(\frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \right) \; + \lambda \|\mathbf{w}\|_2^2$$

Other regularizers

- Have discussed l2 and l1 regularizers

- Other examples:
  - elastic net regularization is a combination of l1 and l2 (i.e., l1 + l2): ensures a unique solution
  - capped regularizers: do not prevent large weights

Does this regularizer still protect against overfitting?



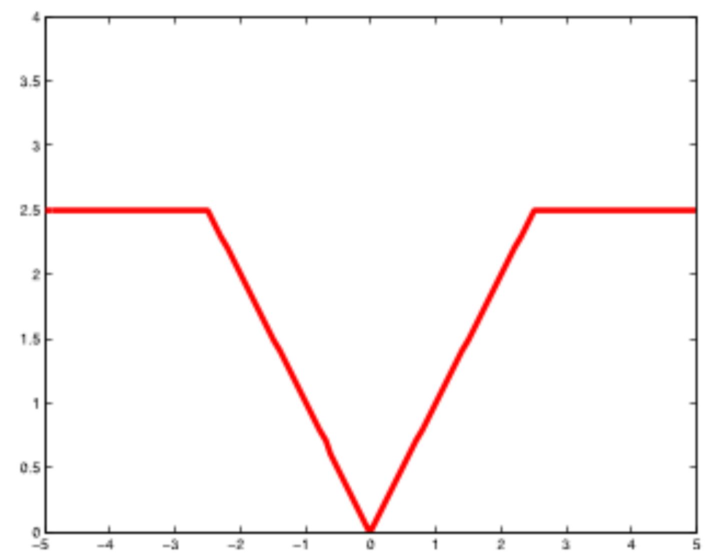
(a) Capped ℓ_1-norm loss ($\varepsilon = 2.5$)

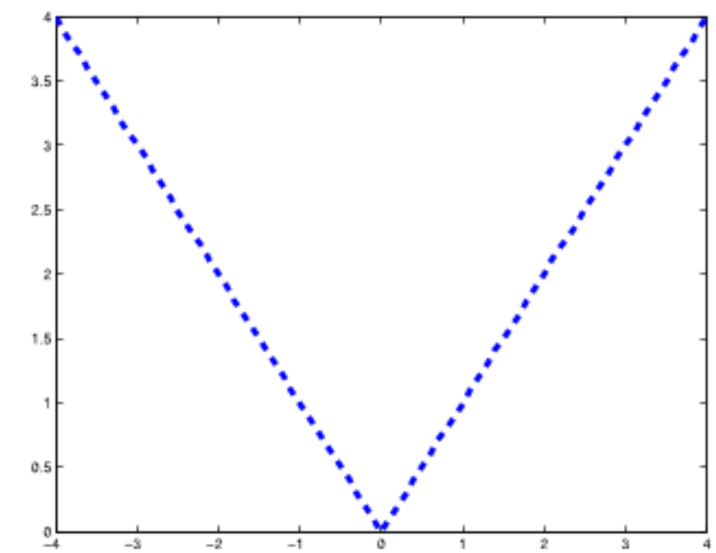
(b) ℓ_1-norm loss

* Figure from "Robust Dictionary Learning with Capped l1-Norm", Jiang et al., IJCAI 2015

Practical considerations: outliers

- What happens if one sample is bad?
- Regularization helps a little bit
- Can also change losses
- Robust losses
  - use l1 instead of l2
  - even better: use capped l1
- What are the disadvantages to these losses?



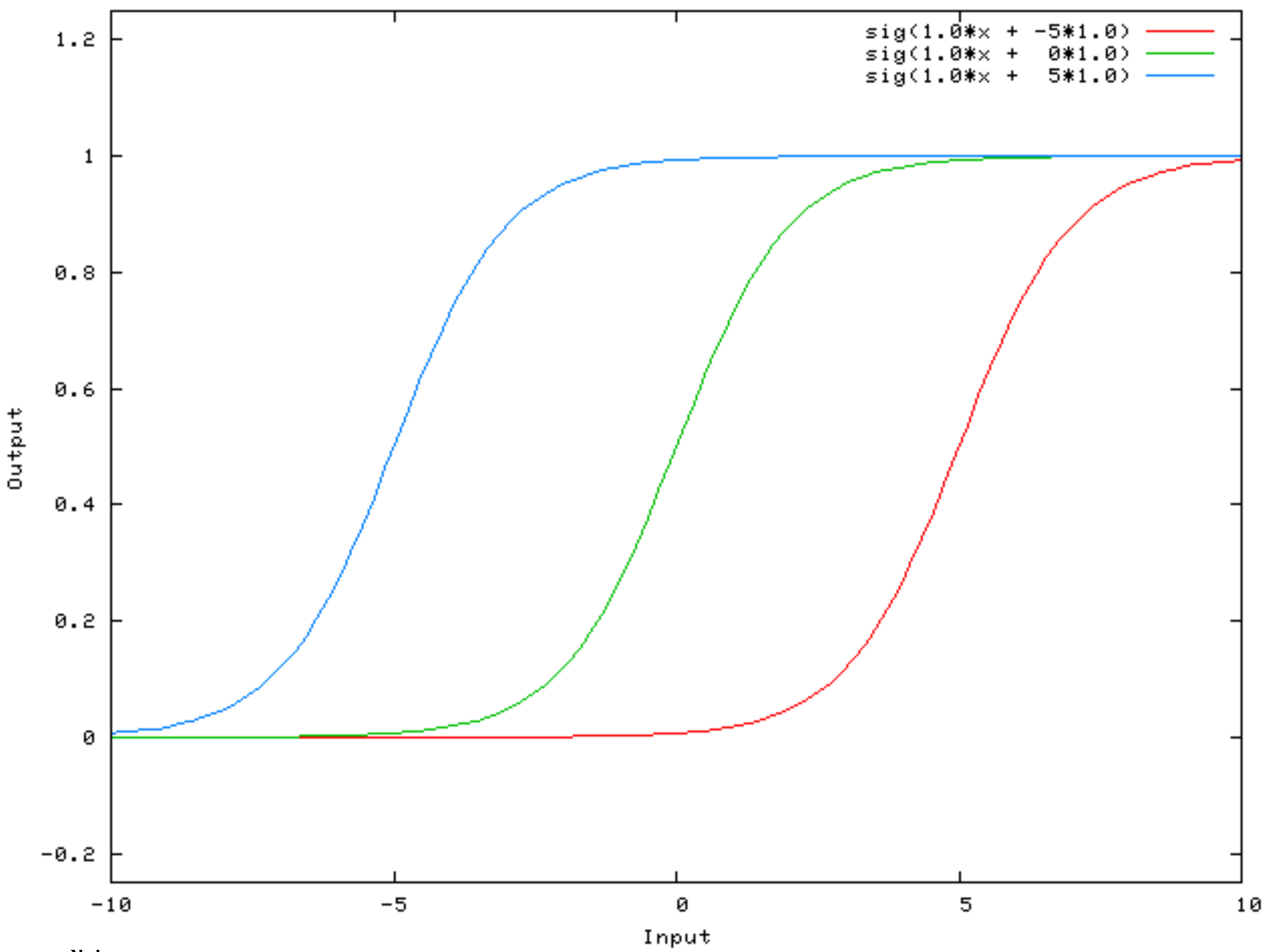


Exercise: intercept unit

- In linear regression, we added an intercept unit (bias unit) to the features
  - i.e., added a feature that is always 1 to the feature vector
- Does it make sense to do this for GLMs?
  - e.g., sigmoid(<x,w> + w_0)

Adding a column of ones to GLMs

- This provides the same outcome as for linear regression
- g(E[y l x]) = x w —> bias unit in x with coefficient w0 shifts the function left or right



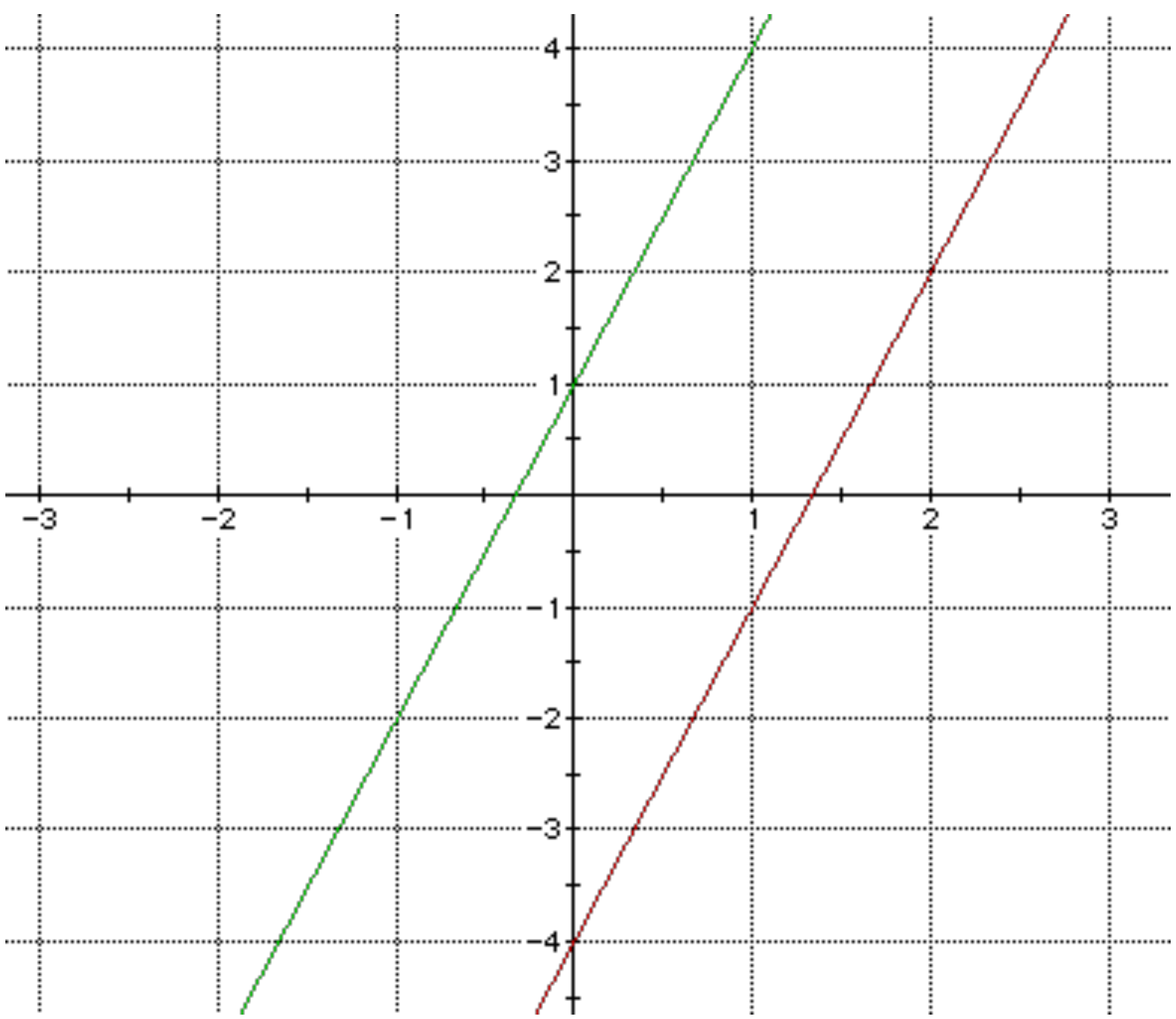


*Figure from http://stackoverflow.com/questions/2480650/role-of-bias-in-neural-networks