Machine Learning

4771

Instructor: Itsik Pe’er

Reminder: Parameter Estimation

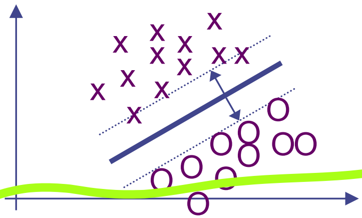
A-Posteriori → Regularization

$$R_{regularized}(\theta) = \frac{1}{N}\sum_{i=1}^{N} Loss(y_i, f(x_i;\theta)) + \frac{\lambda}{2}||\theta||^2$$

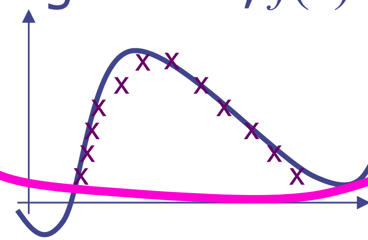
$$\theta^* = (\boldsymbol{X}^T\boldsymbol{X} + \lambda N I)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Regression

Classification

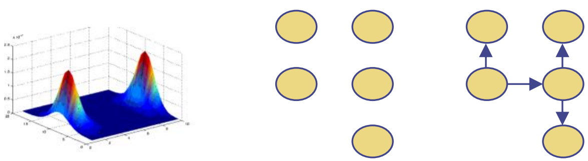


Regression, $f(x)=y$

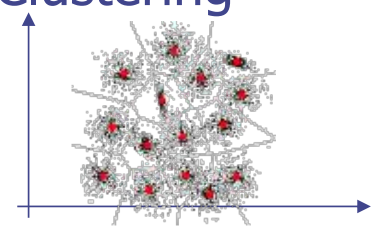


Supervised

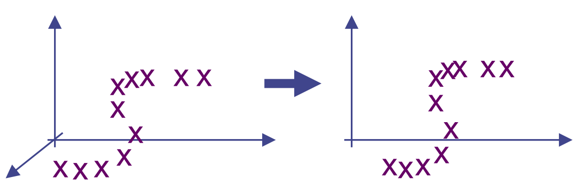
Density/Structure Estimation



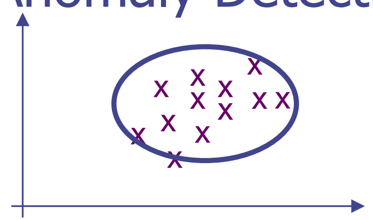
Clustering



Feature Selection



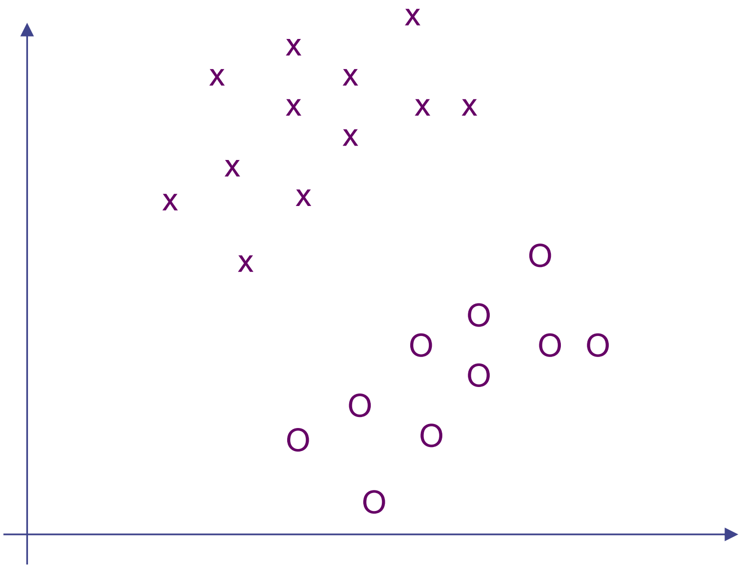
Anomaly Detection



Unsupervised

Class 6

- **Classification**
- Logistic Regression
- Gradient Descent



Classification Problems

- Determine student admission to Columbia based on GPA, prev. school rank, tests

Classification Problems

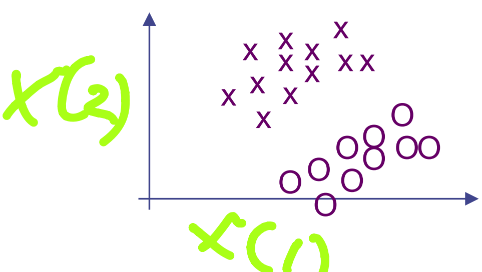
- Determine student admission to Columbia based on GPA, prev. school rank, tests
- Decide malignant or benign tumors based on size, density, speed of growth

Kim et al. '07

Formalizing Classification

- Classification is another important learning problem

Classification: $X = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_N, y_N)\}, \boldsymbol{x}_i \in \boldsymbol{R}^D, y_i \in \{0,1\}$



Classification is like Regression

- Classification is another important learning problem

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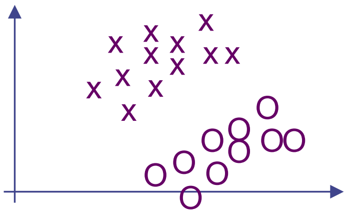
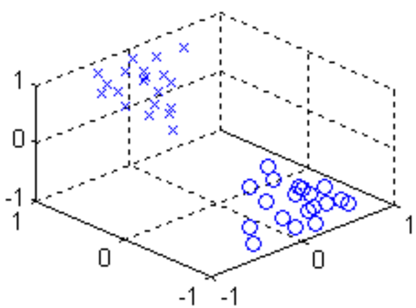
Regression: $X = \{(\boldsymbol{x}_1, t_1), (\boldsymbol{x}_2, t_2), \ldots, (\boldsymbol{x}_N, t_N)\}, \boldsymbol{x}_i \in \boldsymbol{R}^D, t_i \in \boldsymbol{R}$





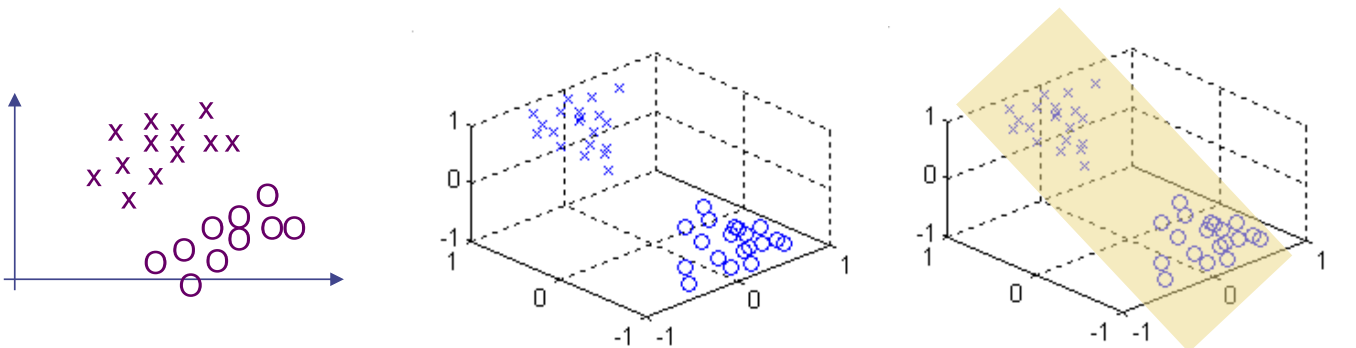
Classification is like Regression

- Classification is another important learning problem

Classification: $X = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_N, y_N)\}, \boldsymbol{x}_i \in \boldsymbol{R}^D, y_i \in \{0,1\}$

Regression: $X = \{(\boldsymbol{x}_1, t_1), (\boldsymbol{x}_2, t_2), \dots, (\boldsymbol{x}_N, t_N)\}, \boldsymbol{x}_i \in \boldsymbol{R}^D, t_i \in \boldsymbol{R}$

- Should we solve this as a least squares regression problem?



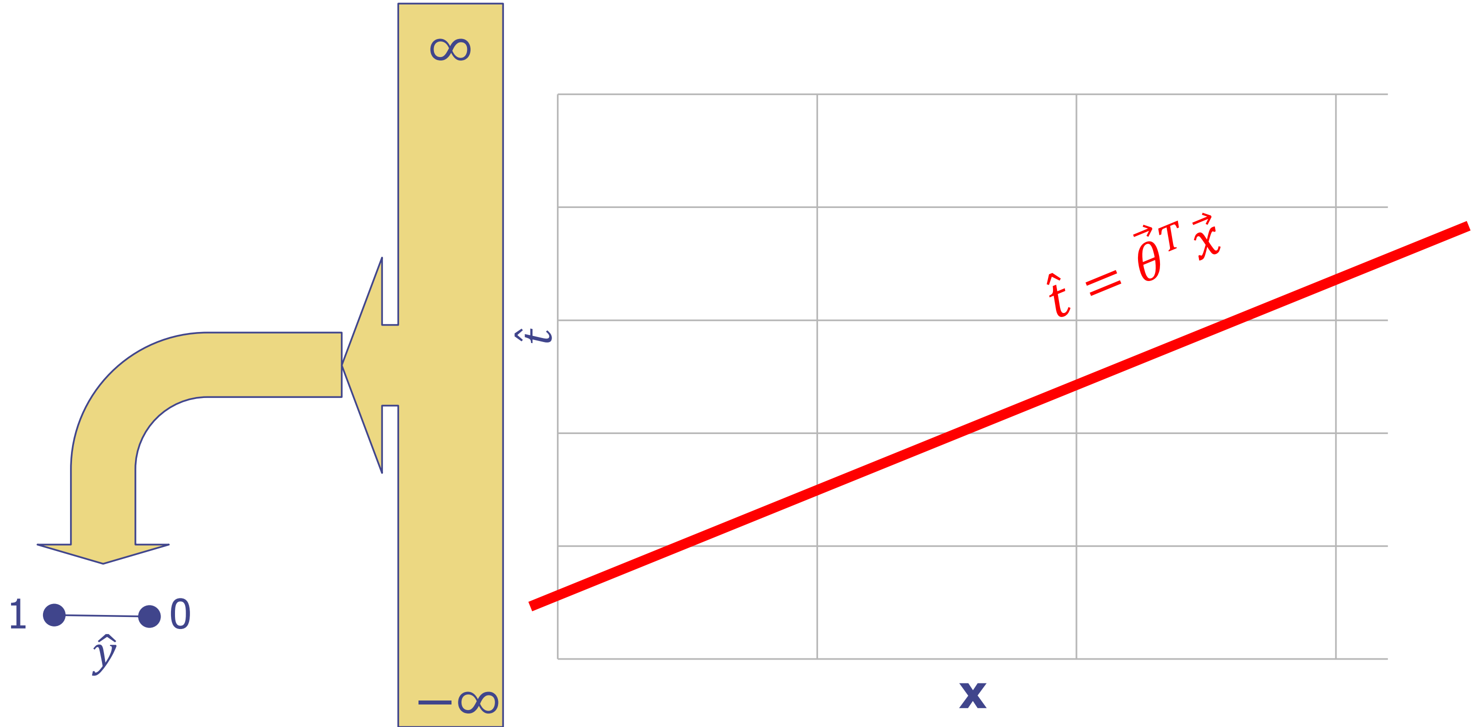
Short hand for Linear Functions

- Hiding the intercept by notation

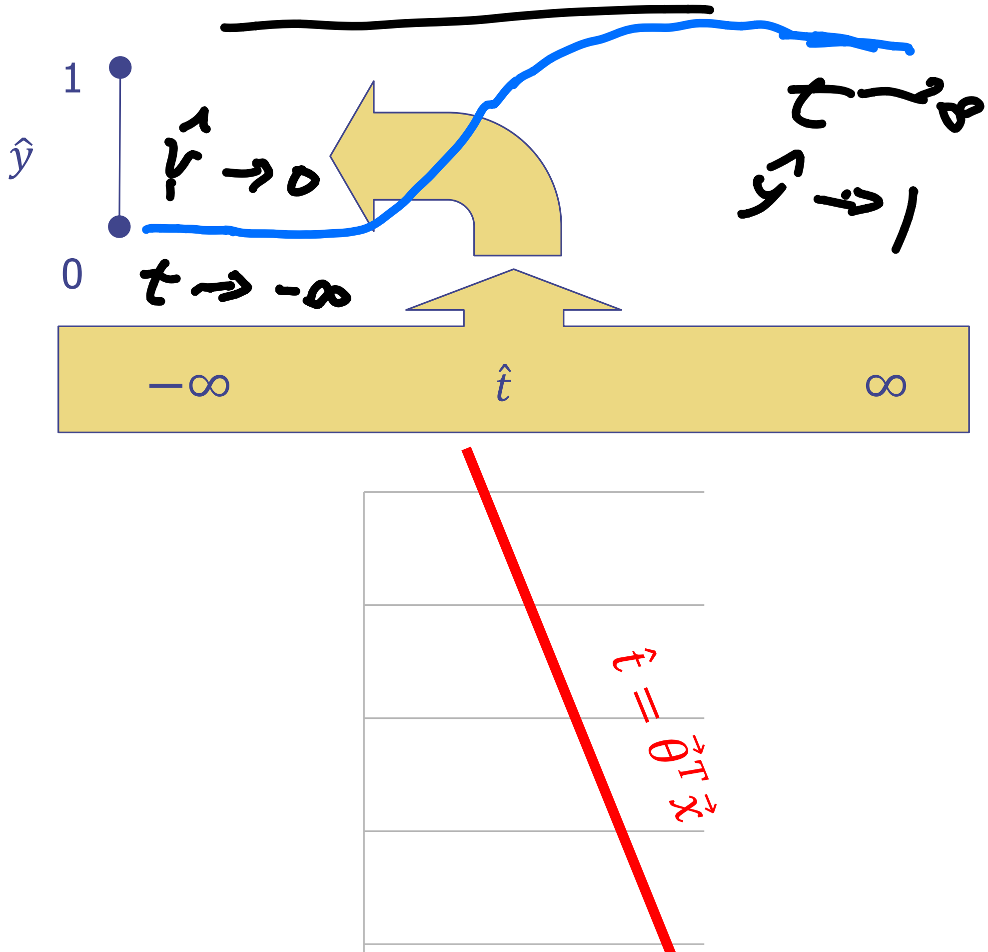
$$f(\boldsymbol{x};\theta) = \theta^T\boldsymbol{x} + \theta_0$$

$$= \begin{bmatrix} \theta(1) \\ \theta(2) \\ \vdots \\ \theta(D) \end{bmatrix} \begin{bmatrix} \boldsymbol{x}(1) \\ \boldsymbol{x}(2) \\ \vdots \\ \boldsymbol{x}(D) \end{bmatrix} + \theta_0 = \begin{bmatrix} \theta_0 \\ \theta(1) \\ \theta(2) \\ \vdots \\ \theta(D) \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{x}(1) \\ \boldsymbol{x}(2) \\ \vdots \\ \boldsymbol{x}(D) \end{bmatrix} = \vec{\theta}^T\vec{\boldsymbol{x}}$$

Recalibrating Range



Recalibrating Range



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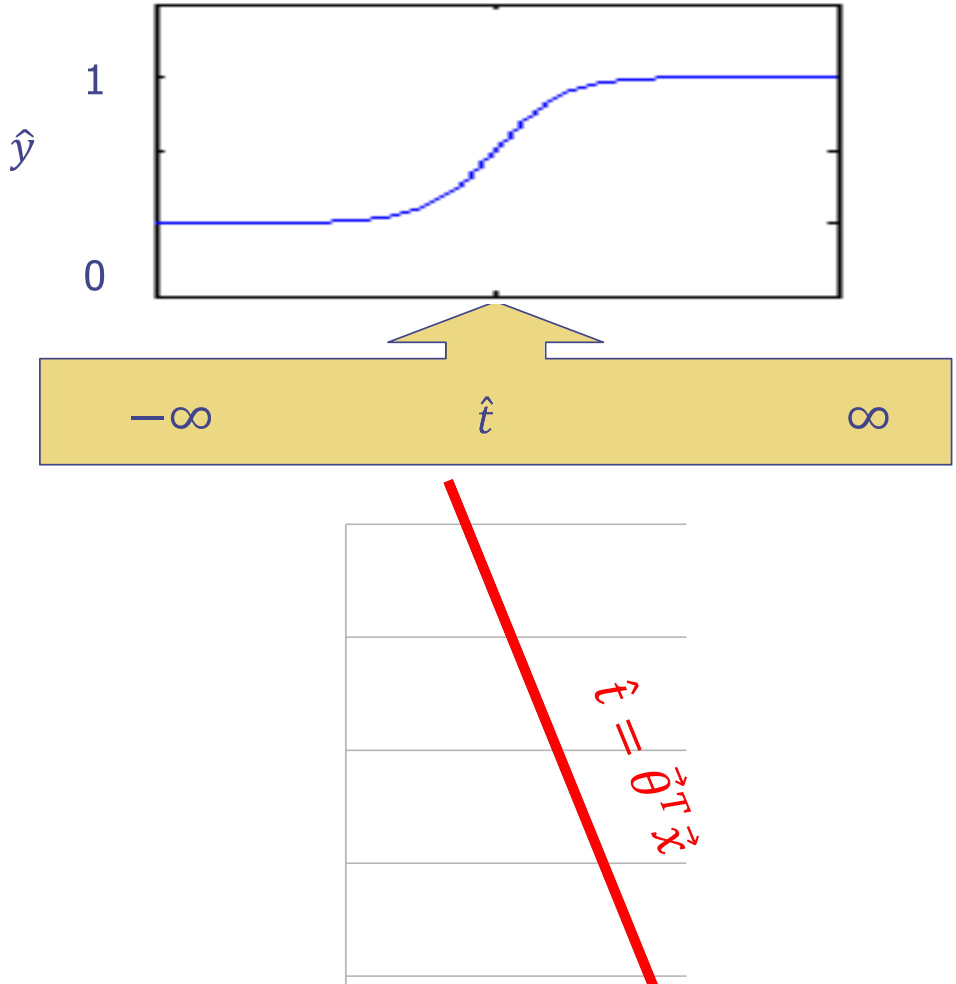

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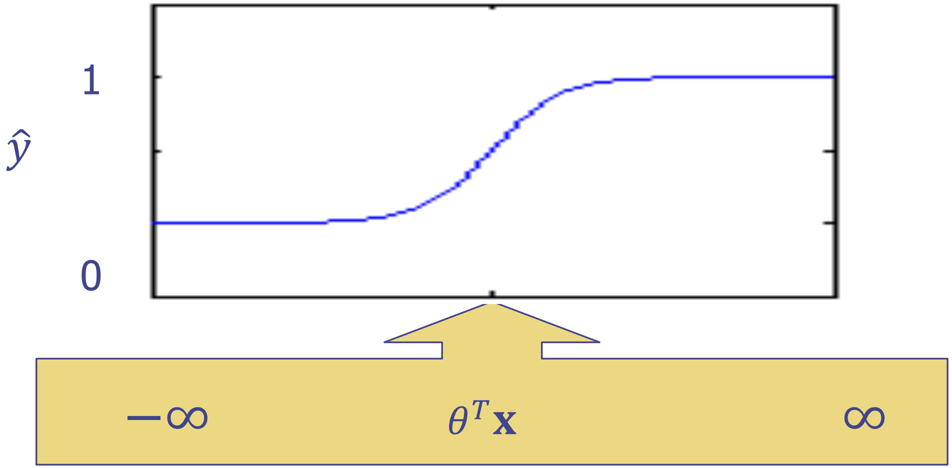


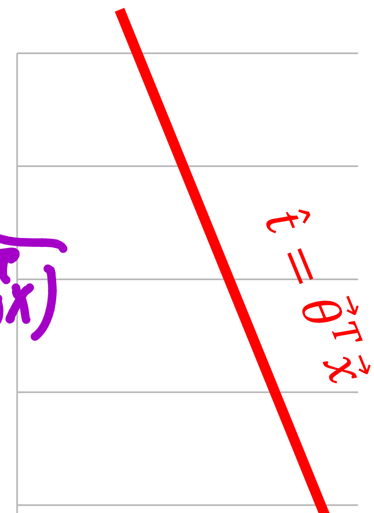
$$\lim_{\theta^T x \to \infty} \hat{y} = 1$$

$$\approx 1 - \exp(-\theta^T x)$$

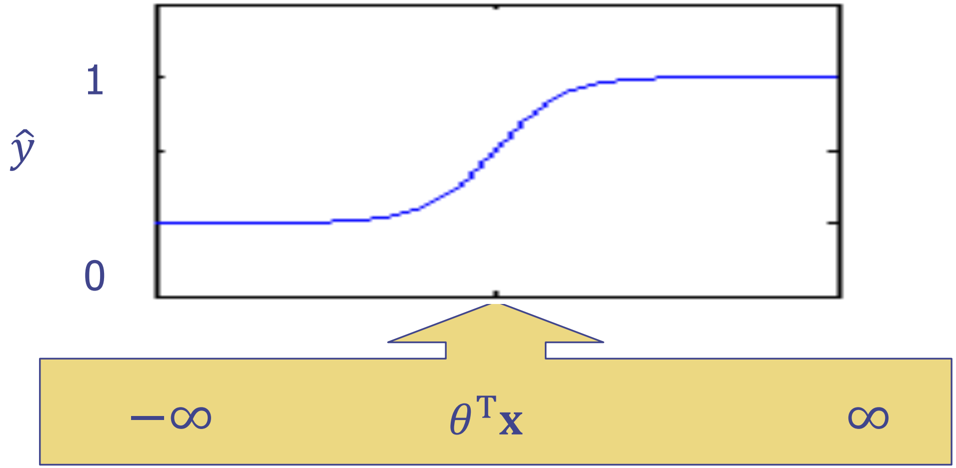
$$\frac{1}{1+\exp(-\theta^T x)}$$

$$\lim_{\theta^T x \to -\infty} \hat{y} = 0$$

$$\approx \exp(\theta^T x)$$



Recalibrating Range



$$\lim_{\theta^T \boldsymbol{x}\to\infty} \hat{y} = 1$$

$$\hat{Y} \underset{\theta^T \boldsymbol{x}\to\infty}{\cong} 1 - \exp(-\theta^T \boldsymbol{x})$$

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$$\hat{Y} \underset{\theta^T \boldsymbol{x}\to-\infty}{\cong} \exp(\theta^T \boldsymbol{x})$$

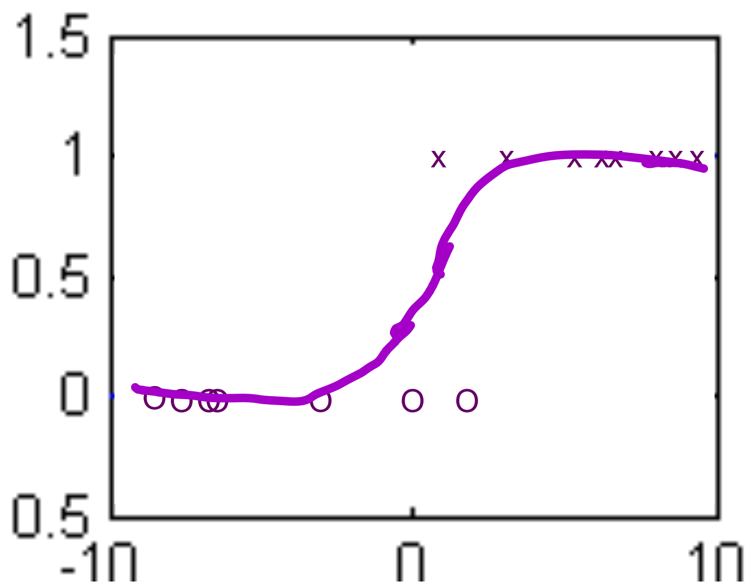
Logistic Regression

- Given a classification problem with binary outputs

$$X = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_N, y_N)\}, \boldsymbol{x}_i \in \boldsymbol{R}^D, y_i \in \{0,1\}$$

- Use this function and output 1 if $f(\boldsymbol{x}) > 0.5$ and 0 otherwise

$$f(\boldsymbol{x}; \theta) = \frac{1}{1 + exp(-\theta^T \boldsymbol{x})}$$



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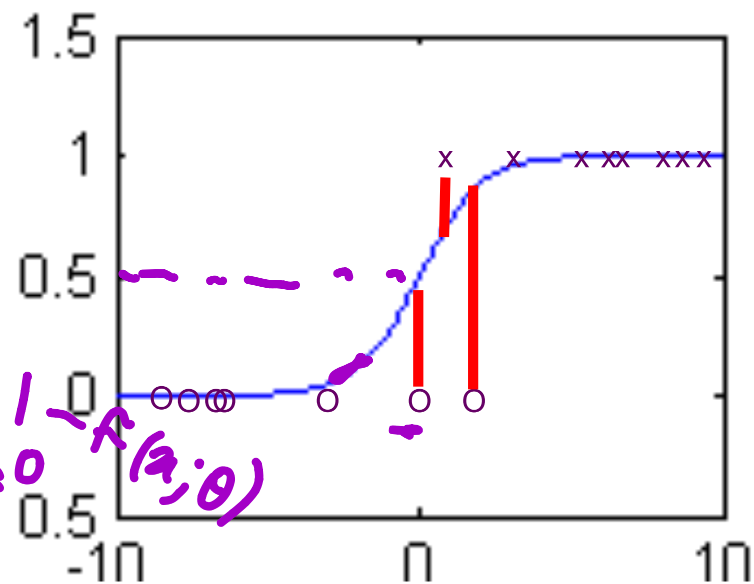
$$f(\boldsymbol{x};\theta) = \frac{1}{1 + exp(-\theta^T \boldsymbol{x})}$$

$$Pr(y=1) = f(x;\theta)$$

$$-\log Pr(y_i | f(x_i;\theta)) \rightarrow 1 - f(x_i;\theta)$$

$$\text{if } y_i = 1: f(x_i;\theta) \qquad \text{if } y_i = 0$$



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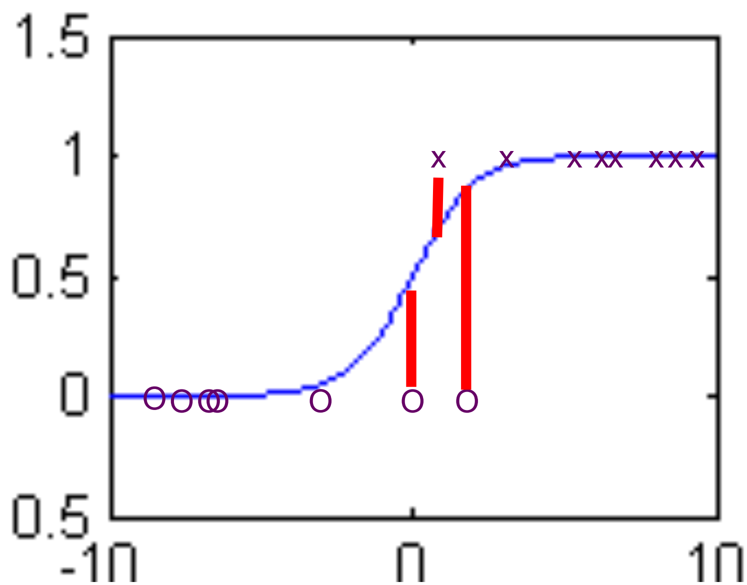
- Assume $\Pr(y = 1) = f(\boldsymbol{x};\theta)$



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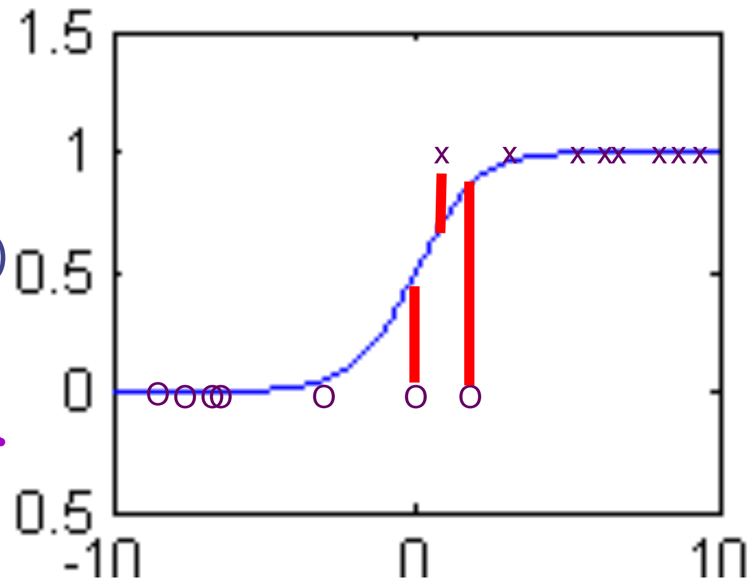
Log

- $\Pr(y | f(\boldsymbol{x}; \theta)) =$

$= \cancel{\Pi}_{y_i=0}(1 - f(\boldsymbol{x}_i; \theta)) \cancel{\Pi}_{y_i=1} f(\boldsymbol{x}_i; \theta)$

Σ log $\uparrow$ Σ log $\uparrow$

$\Sigma (1-y_i) \log (1-f) + \Sigma y_i \cdot \log f$



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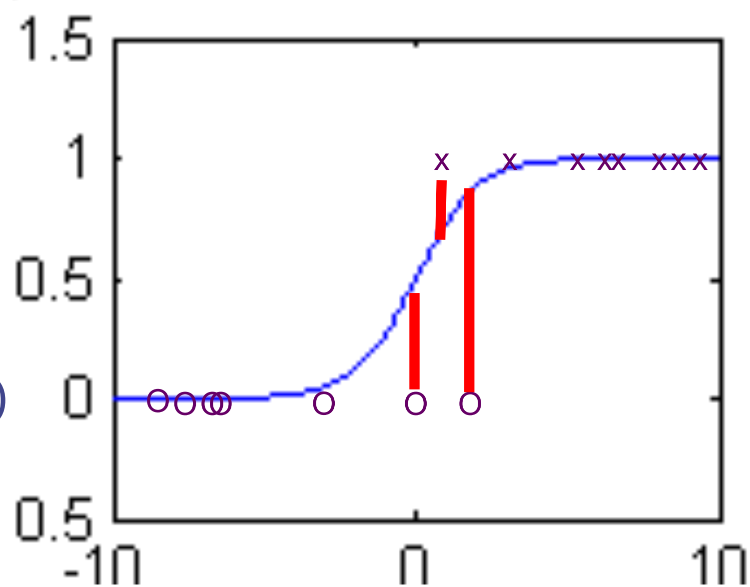

- Assume $\Pr(y_i = 1) = f(\boldsymbol{x}_i; \theta)$

- $\Pr(y | f(\boldsymbol{x}; \theta)) =$
$= \prod_{y_i=0} \left(1 - f(\boldsymbol{x}_i; \theta)\right) \prod_{y_i=1} f(\boldsymbol{x}_i; \theta)$

- $\log \Pr(y | f(\boldsymbol{x}; \theta)) =$
$= \sum_i \left[y_i \log f(\boldsymbol{x}_i; \theta) + (1 - y_i) \log\left(1 - f(\boldsymbol{x}_i; \theta)\right) \right]$

Logistic Regression

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$$f(\boldsymbol{x};\theta) = \frac{1}{1 + exp(-\theta^T \boldsymbol{x})}$$

- Instead of squared loss, use Logistic Loss (i.e. negative binomial likelihood)

$$Loss_{log}\big(y, f(\boldsymbol{x};\theta)\big) = (y-1)\log\big(1 - f(\boldsymbol{x};\theta)\big) - y\log(f(\boldsymbol{x};\theta))$$

- The resulting method is called Logistic Regression.
- Empirical Risk:

Logistic Regression

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- Empirical Risk:

$$R_{emp}(\theta) = \frac{1}{N}\sum_{i=1}^{N}\Big[(y_i - 1)\log\big(1 - f(\boldsymbol{x}_i; \theta)\big) - y_i\log(f(\boldsymbol{x}_i; \theta))\Big]$$

Logistic Regression

- With empirical logistic risk has no closed form solution:

$$R_{emp}(\theta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - 1)\log\big(1 - f(\boldsymbol{x_i};\theta)\big) - y_i \log(f(\boldsymbol{x_i};\theta))$$

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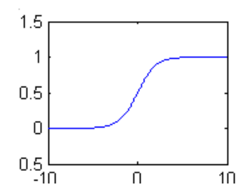

$$D_\theta f(x;\theta) = \frac{1}{(1 + \exp(-\theta^T x))} \cdot \frac{\exp(-\theta^T x)}{1 + \exp(-\theta^T x)} x$$

Logistic Regression

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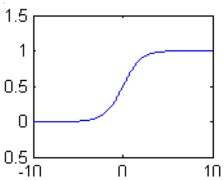
$$R_{emp}(\theta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - 1)\log\big(1 - f(\boldsymbol{x_i};\theta)\big) - y_i\log(f(\boldsymbol{x_i};\theta))$$

$$\nabla_\theta R = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{1-y_i}{1-f(\boldsymbol{x_i};\theta)} - \frac{y_i}{f(\boldsymbol{x_i};\theta)}\right)f'(\boldsymbol{x_i};\theta) = 0 \quad ??????$$

where

$$f(\boldsymbol{x};\theta) = \frac{1}{1+exp(-\theta^T\boldsymbol{x})} = g(\theta^T\boldsymbol{x})$$

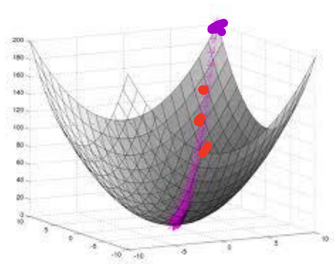
Find best θ numerically!



$$g(z) = \frac{1}{1+exp(-z)} \qquad g'(z) = g(z)(1-g(z))$$

Gradient Descent

- Useful when we can't get minimum solution in closed form
- Gradient points in direction of fastest increase
- Take step in the opposite direction!



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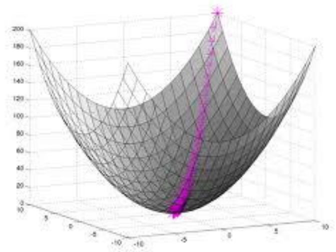


- Gradient Descent Algorithm

choose scalar step size η, *& tolerance* ε
initialize θ^0 *= small random vector*

$$\theta^1 \leftarrow \theta^0 - \eta_0 \nabla_\theta R_{emp}|_{\theta^0} \ ; t \leftarrow 1$$

while $\|\theta^t - \theta^{t-1}\| \geq \epsilon$ *{*

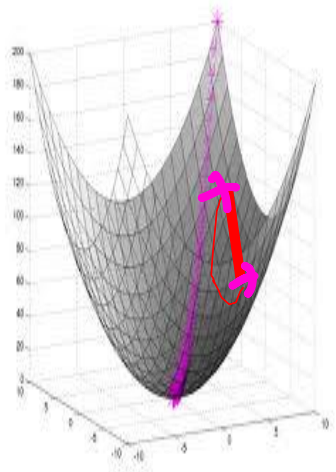
$$\theta^{t+1} \leftarrow \theta^t - \eta_t \nabla_\theta R_{emp}|_{\theta^t} \ ; t \leftarrow t+1 \ \}$$

- For appropriate $\{\eta_t\}$, this will converge to local minimum

Gradient Descent Convergence

$$R_{emp}(\theta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - 1)\log\big(1 - f(\boldsymbol{x_i};\theta)\big) - y_i\log(f(\boldsymbol{x_i};\theta))$$

is a convex function, so local minimum is global



Gradient Descent Convergence

$$R_{emp}(\theta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - 1)\log\big(1 - f(\boldsymbol{x}_i;\theta)\big) - y_i\log(f(\boldsymbol{x}_i;\theta))$$

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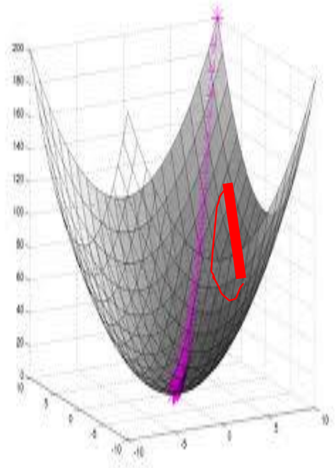
Proof:

Convex combination of
 convex functions
$-\log\big(1 - f(\boldsymbol{x}_i;\theta)\big)$ and $-\log(f(\boldsymbol{x}_i;\theta))$



Convexity of Regression Loss

∇_θ $-\log(f(\boldsymbol{x}_i;\theta))$ is a convex function

$$\nabla_\theta \left[\cancel{-f}(x_i, \tfrac{1}{1+\exp(-\theta^T x_i)}) \right] = \frac{-\exp(-\theta^T x_i)\cdot x_i}{1+\exp(-\theta^T x_i)}$$

Convexity of Regression Loss

$-\log(f(\boldsymbol{x}_i;\theta))$ is a convex function

Proof:

$$\nabla_\theta^{2}\left[-\log\left(f(\boldsymbol{x}_i;\theta)\right)\right] =$$

$$= \nabla_\theta\left[-\log\left(\frac{1}{1+\exp(-\theta^T x_i)}\right)\right]$$

$$= \nabla_\theta[\log(1+\exp(-\theta^T x_i))]$$

$$= \frac{-\exp(-\theta^T x_i)\,x_i}{1+\exp(-\theta^T x_i)} = \nabla\left[\frac{1}{1+\exp(-\theta^T x_i)}-1\right]$$

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

Convexity of Regression Loss

$-\log(f(\boldsymbol{x}_i;\theta))$ is a convex function

Proof:

$$\nabla_\theta^2\left[-\log\left(f(\boldsymbol{x}_i;\theta)\right)\right]$$

$$= \nabla_\theta\left[\left(\frac{1}{1+\exp(-\theta^T x_i)} - 1\right)x_i\right] =$$

$$= \frac{1}{1+\exp(-\theta^T x)} \cdot \frac{\exp(-\theta^T x)}{1+\exp(-\theta^T x)} x_i x_i^T$$

Convexity of Regression Loss

$-\log(f(\boldsymbol{x}_i;\theta))$ is a convex function

Proof:

$$\nabla_\theta^2\left[-\log\left(f(\boldsymbol{x}_i;\theta)\right)\right]$$

$$= \nabla_\theta\left[\left(\frac{1}{1+\exp(-\theta^T x_i)} - 1\right)x_i\right]$$

$$= \frac{1}{1+\exp(-\theta^T x_i)}\frac{\exp(-\theta^T x_i)}{1+\exp(-\theta^T x_i)}x_i x_i^T$$

Convexity of Regression Loss

$-\log(f(\boldsymbol{x}_i;\theta))$ is a convex function

Proof:

$$z^T\,\nabla_\theta^2\left[-\log\left(f(\boldsymbol{x}_i;\theta)\right)\right]z =$$

$$z^T\,\frac{1}{1+\exp(-\theta^T x_i)}\,\frac{\exp(-\theta^T x_i)}{1+\exp(-\theta^T x_i)}\,x_i x_i^T z$$

$$= \frac{1}{1+\exp(-\theta^T x_i)}\,\frac{\exp(-\theta^T x_i)}{1+\exp(-\theta^T x_i)}\left(x_i^T z\right)^2$$

Convexity of Regression Loss

$\nabla_\theta -\log(1 - f(\boldsymbol{x}_i; \theta))$ is a convex function

$$\nabla_\theta - \log \frac{\exp(-\theta^T x)}{1 + \exp(\theta^T x)}$$

$$\nabla_\theta \theta^T x + \nabla_\theta \log(1 + \exp \theta^T x)$$

Convexity of Regression Loss

$-\log(1 - f(\boldsymbol{x}_i;\theta))$ is a convex function

Proof:

$$\nabla_\theta\left[-\log\left(1 - f(\boldsymbol{x}_i;\theta)\right)\right] =$$

$$= \nabla_\theta\left[-\log\left(\frac{\exp(-\theta^T x_i)}{1 + \exp(-\theta^T x_i)}\right)\right]$$

$$= \nabla_\theta[\theta^T x_i + \log(1 + \exp(-\theta^T x_i))]$$

$$= x_i + \nabla_\theta[\log(1 + \exp(-\theta^T x_i))]$$

Convexity of Regression Loss

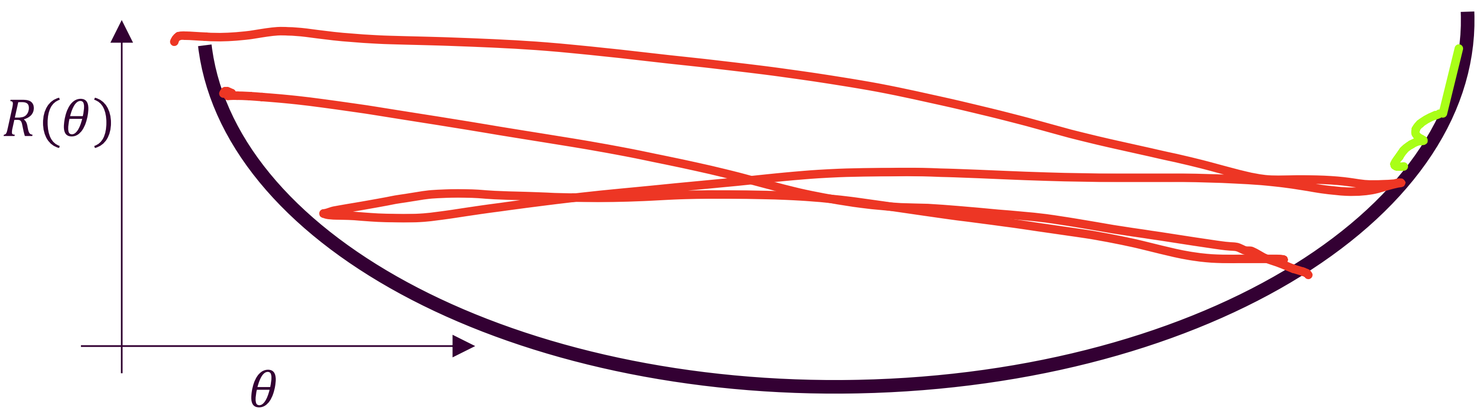
$-\log(1 - f(\boldsymbol{x}_i; \theta))$ is a convex function

Proof:

$$\nabla_\theta^2 \left[-\log\left(1 - f(\boldsymbol{x}_i; \theta)\right) \right] =$$

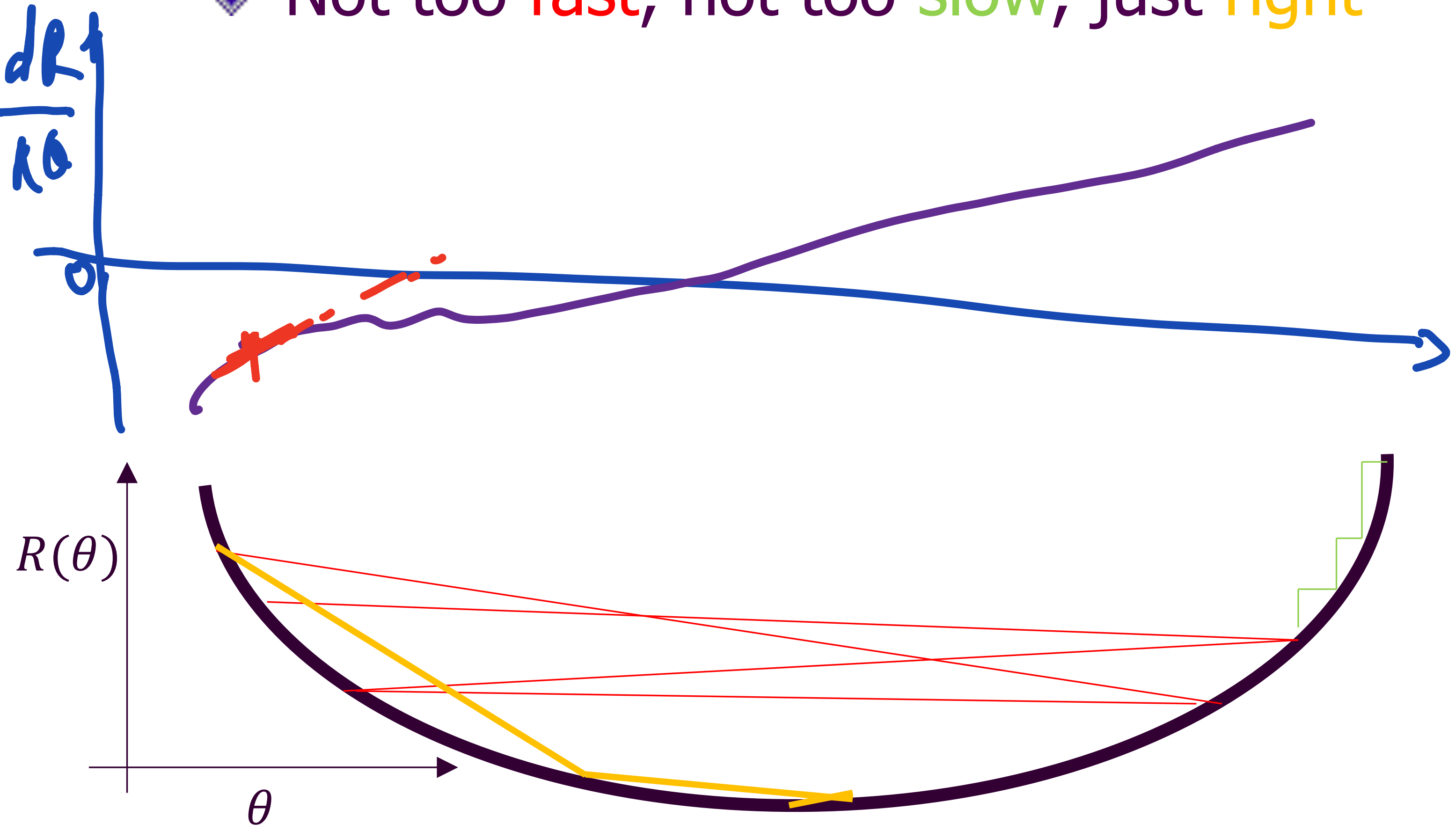
$$= \nabla_\theta^2 \left[\log(1 + \exp(-\theta^T x_i)) \right]$$

How fast to descend?



How fast to descend?

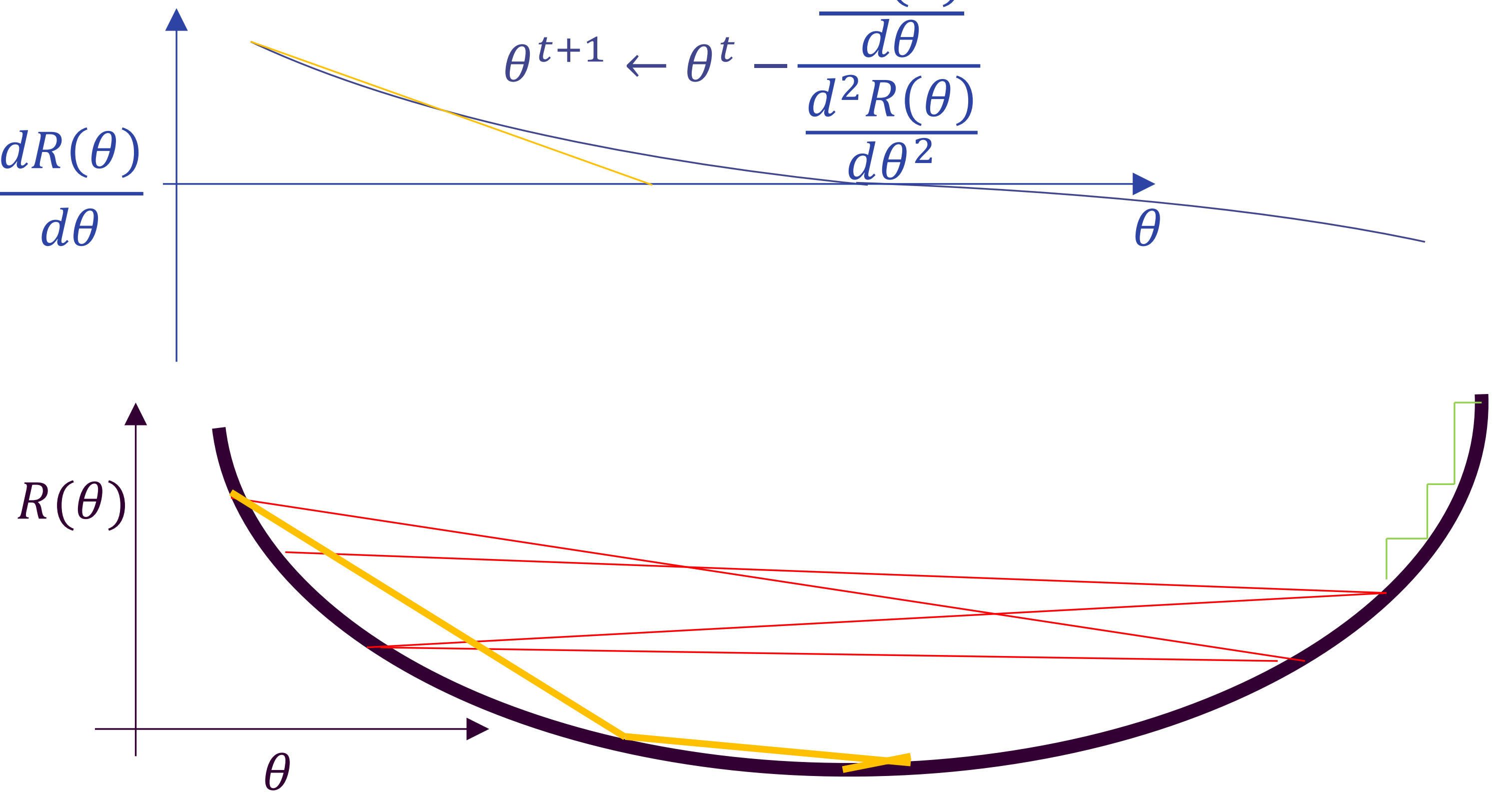
- Not too fast, not too slow, just right



How fast to descend?

- Newton's method for the derivative

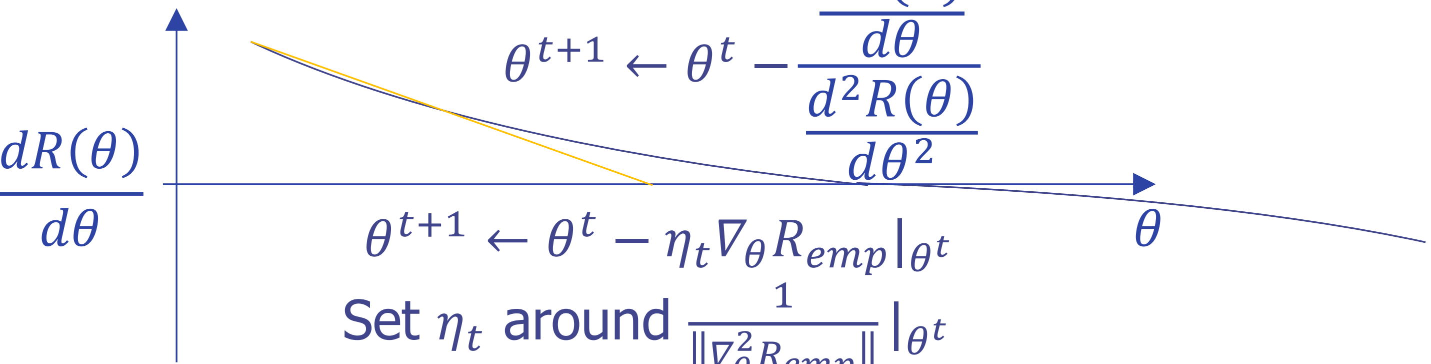
$$\theta^{t+1} \leftarrow \theta^{t} - \frac{\frac{dR(\theta)}{d\theta}}{\frac{d^2R(\theta)}{d\theta^2}}$$



How fast to descend?

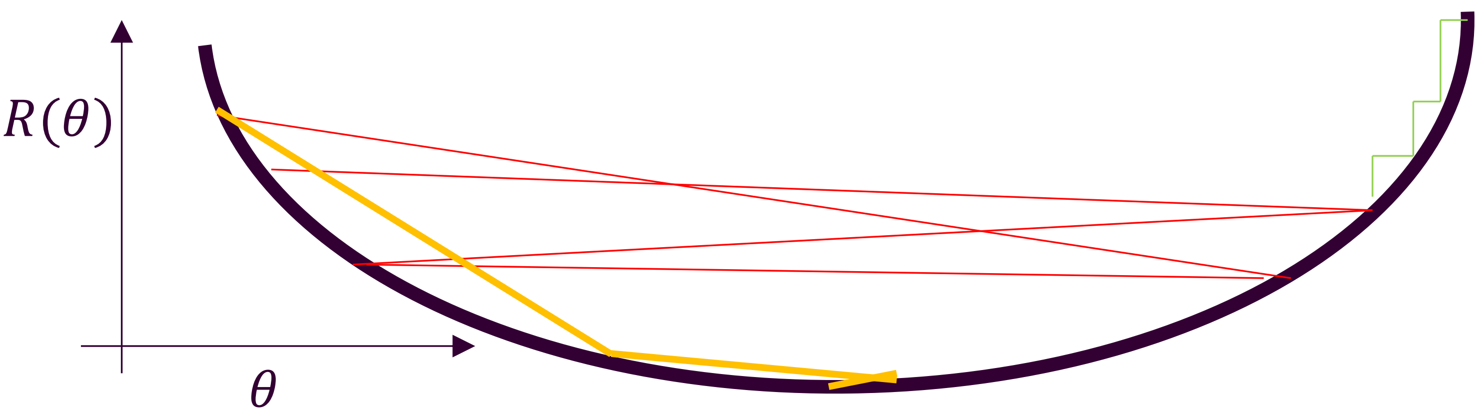
- Newton's method for the derivative

$$\theta^{t+1} \leftarrow \theta^{t} - \frac{\frac{dR(\theta)}{d\theta}}{\frac{d^2R(\theta)}{d\theta^2}}$$



$$\theta^{t+1} \leftarrow \theta^{t} - \eta_t \nabla_\theta R_{emp}|_{\theta^t}$$

Set η_t around $\frac{1}{\|\nabla_\theta^2 R_{emp}\|}|_{\theta^t}$



Summary

- Classification
- Logistic Regression
- Gradient Descent