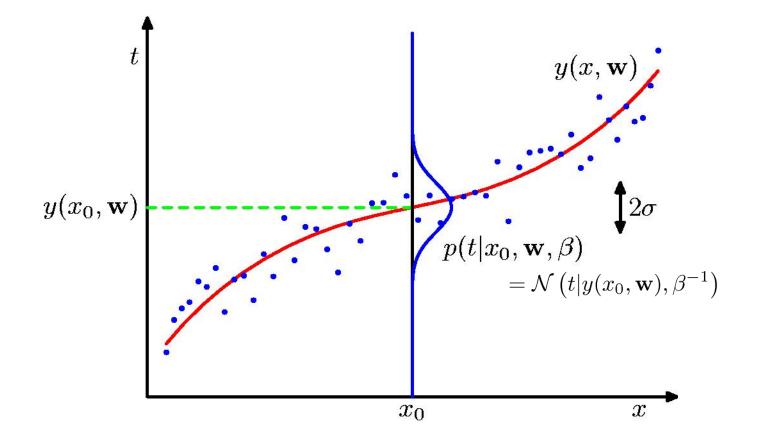
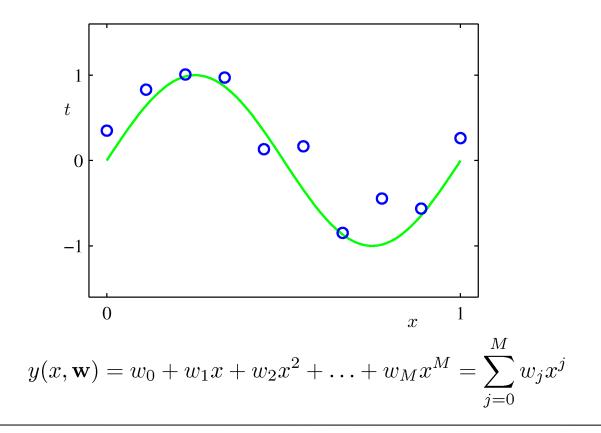
#### **Curve Fitting Re-visited**



#### Linear Basis Function Models (1)

#### **Example: Polynomial Curve Fitting**



#### Linear Basis Function Models (2)

#### Generally

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

Where  $\phi_j(x)$  are known as *basis functions*. Typically,  $\phi_0(x) = 1$ , so that  $W_0$  acts as a bias. In the simplest case, we use linear basis functions :  $\phi_d(x) = x_d$ .

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$
  

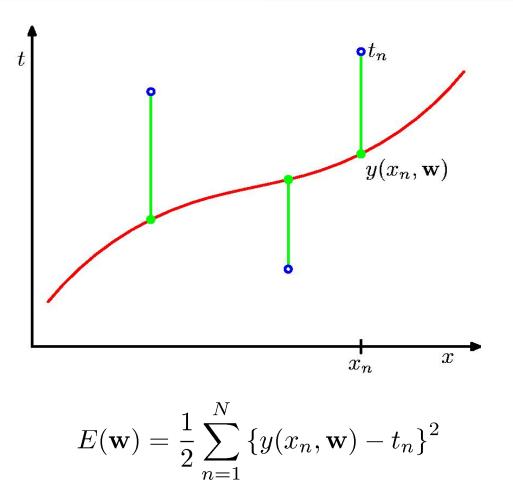
$$\mathbf{Data} \quad \begin{array}{l} \mathbf{x} = (x_1, \dots, x_N)^{\mathrm{T}} \\ \mathbf{t} = (t_1, \dots, t_N)^{\mathrm{T}} \end{array}$$
  

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\underbrace{\frac{\beta}{2} \sum_{n=1}^{N} \left\{y(x_n, \mathbf{w}) - t_n\right\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

Determine  $\mathbf{w}_{ML}$  by minimizing sum-of-squares error,  $E(\mathbf{w})$ . Determine also the precision parameter (inverse variance):

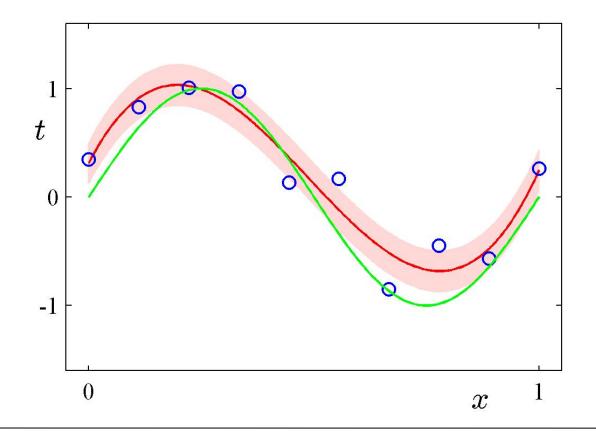
$$\frac{1}{\beta_{\rm ML}} = \frac{1}{N} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}_{\rm ML}) - t_n \}^2$$

#### Sum-of-Squares Error Function



#### **Predictive Distribution**

$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right)$$



#### MAP: A Step towards Bayes

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

$$\beta \widetilde{E}(\mathbf{w}) = \frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

Determine  $\mathbf{w}_{\text{MAP}}$  by minimizing regularized sum-of-squares error,  $\widetilde{E}(\mathbf{w})$ .

#### **Bayesian Curve Fitting**

$$p(t|x, \mathbf{x}, \mathbf{t}) = \int p(t|x, \mathbf{w}) p(\mathbf{w}|\mathbf{x}, \mathbf{t}) \, \mathrm{d}\mathbf{w} = \mathcal{N}\left(t|m(x), s^2(x)\right)$$

Training data

$$\mathbf{x} = (x_1, \dots, x_N)^{\mathrm{T}}$$
  
 $\mathbf{t} = (t_1, \dots, t_N)^{\mathrm{T}}$ 

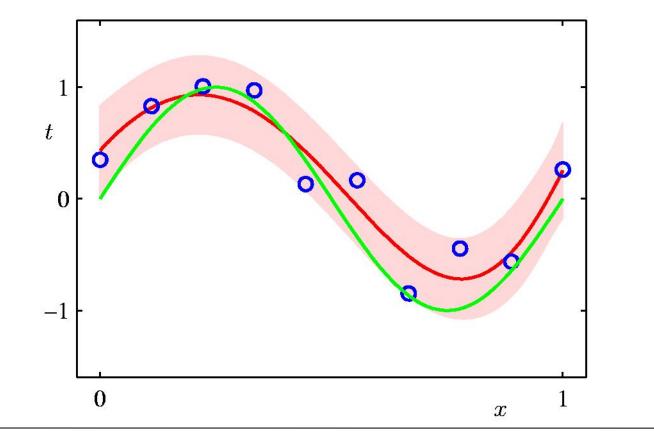
$$m(x) = \beta \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) t_n \qquad s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \boldsymbol{\phi}(x)$$

Where 
$$\mathbf{S}^{-1} = \alpha \mathbf{I} + \beta \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^{\mathrm{T}}$$

E.g. polynomials as basis functions  $oldsymbol{\phi}(x_n) = \left(x_n^0, \dots, x_n^M
ight)^{ ext{T}}$ 

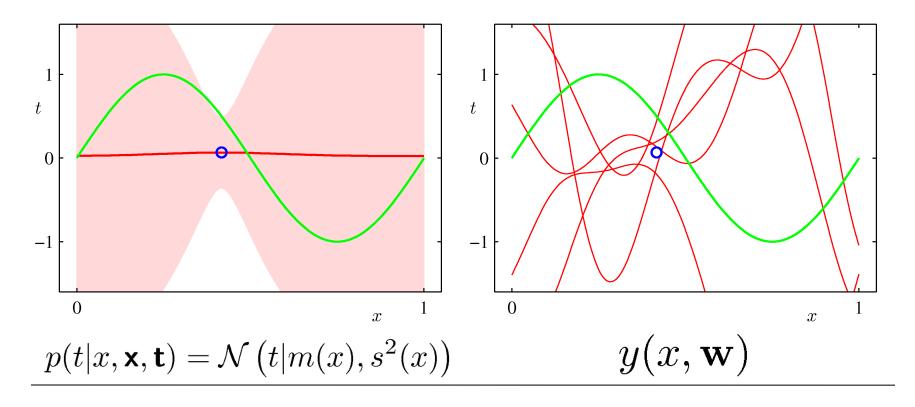
#### **Bayesian Predictive Distribution**

$$p(t|x, \mathbf{x}, \mathbf{t}) = \mathcal{N}\left(t|m(x), s^2(x)\right)$$



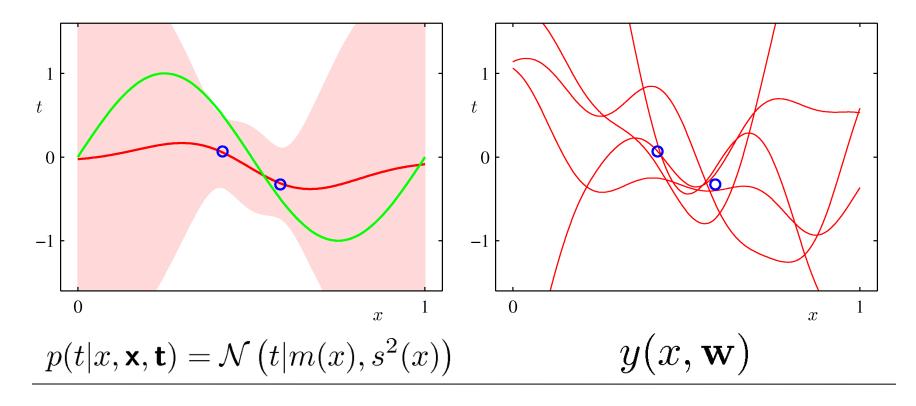
### Predictive Distribution (2)

#### Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point



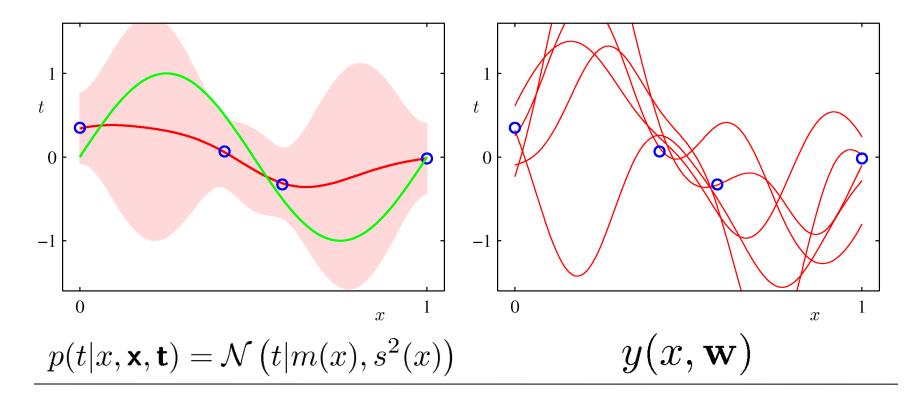
#### Predictive Distribution (3)

# Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points



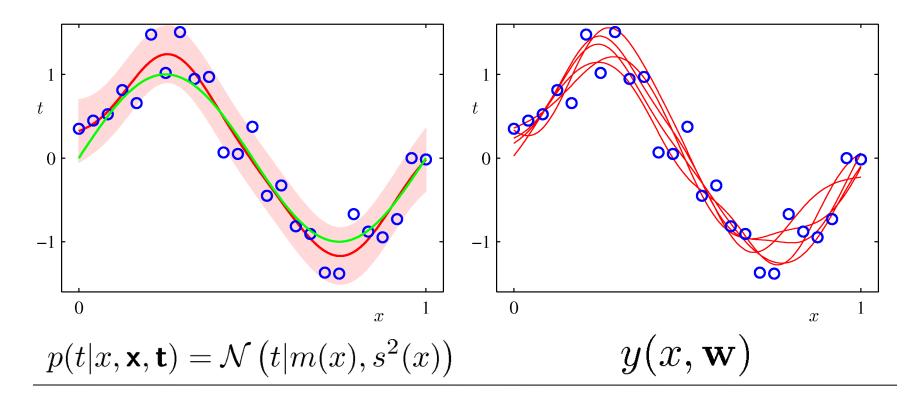
#### **Predictive Distribution (4)**

# Example: Sinusoidal data, 9 Gaussian basis functions, 4 data points



### **Predictive Distribution (5)**

# Example: Sinusoidal data, 9 Gaussian basis functions, 25 data points



#### **Regression vs. Classification**

**Regression:** 

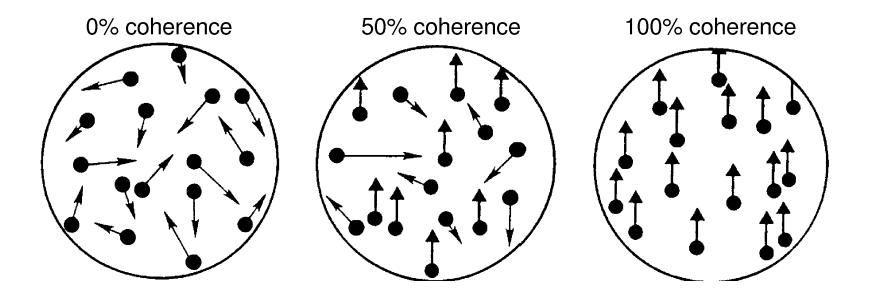
$$x \in [-\infty, \infty], t \in [-\infty, \infty]$$

Classification:

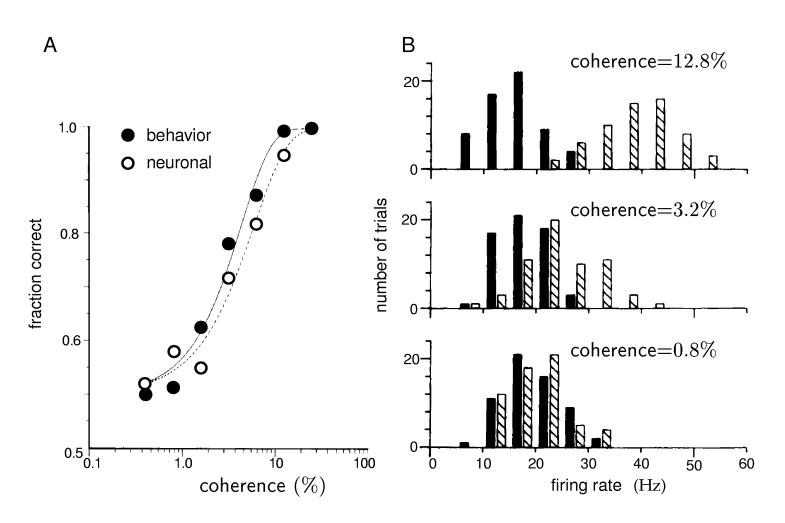
 $x\in [-\infty,\infty], t\in \{0,1\}$ 

## **Neural Example: neuron in MT**

- Middle temporal cortex: large receptive fields sensitive to object motion
- record from single neuron during movement patterns such as the ones below
- animal is trained to decide if the coherent movement is upwards or downwards



- Left: behavioral performance of the animal and of an "ideal observer" considering single neuron
- Right: histograms (thinned) of average firing rate for different stimuli (up/down) at different coherence levels



Optimal strategy for discriminating between two alternative signals presented in background of noise?

Let's call the two alternative signals: + and –

Assume we must base our decisions on the observation of a single observable x x could be e.g. the firing rate of a neuron when x is present

If the signal is + then the values of x are chosen from P(x|+)If the signal is - then the values of x are chosen from P(x|-)

If we have seen a particular value of x, can we tell which signal was presented?

Intuition: Divide x axis at critical point  $x_0$ : Everything to right is called a +, everything to the left a -.

How should we choose  $x_0$ ?

Compute probability of correct decision as function of threshold... ...then find the value of the threshold that maximizes this probability!

Probability of correctly identifying signal +:

$$P(\text{say } + | \text{signal is } +) = \int_{x_0}^{\infty} dx P(x| +)$$

Probability of correctly identifying signal -:

$$P(\text{say -}|\text{signal is -}) = \int_{\infty}^{x_0} dx P(x|-)$$

Probability of making correct choice:

$$P_c(x_0) = P(+) \int_{x_0}^{\infty} dx P(x|+) + P(-) \int_{\infty}^{x_0} dx P(x|-)$$

Probability of making correct choice:

$$P_c(x_0) = P(+) \int_{x_0}^{\infty} dx P(x|+) + P(-) \int_{\infty}^{x_0} dx P(x|-)$$

Maximize it!

$$\frac{dP_c(x_0)}{dx_0} = 0$$

$$P(+)\frac{d}{dx_0}\int_{x_0}^{\infty} dx P(x|+) + P(-)\frac{d}{dx_0}\int_{\infty}^{x_0} dx P(x|-) = 0$$

$$-P(+) P(x_0|+) + P(-)P(x_0|-) = 0$$

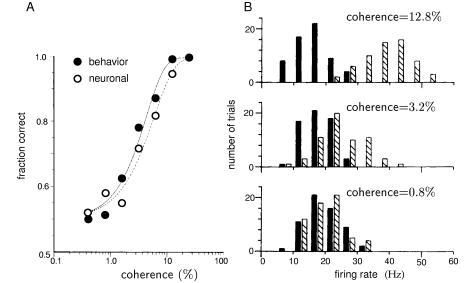
 $P(+) P(x_0|+) = P(-)P(x_0|-)$ 

$$P(+)P(x_0|+) = P(-)P(x_0|-)$$

In the simple case that signals x and – are equally likely, i.e. P(+)=P(-)

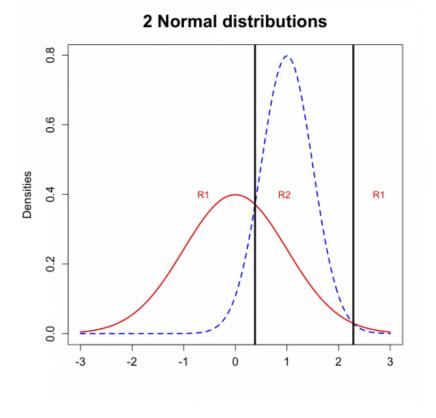
$$P(x_0|+) = P(x_0|-)$$

Set threshold where two probabilities cross



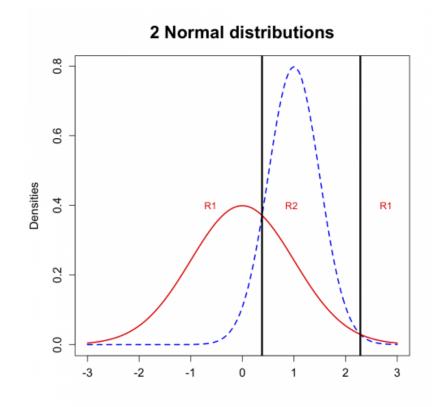
$$P(x_0|+) = P(x_0|-)$$

There can be several dividing lines

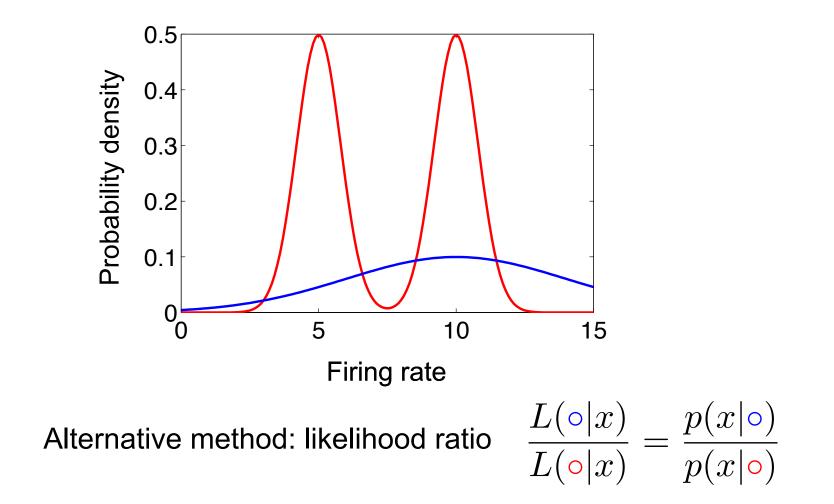


In general: One cannot do better than the likelihood ratio

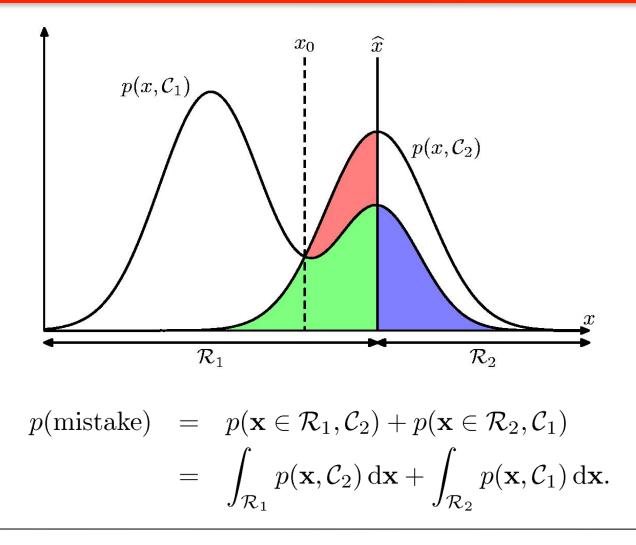
$$l(x) = \frac{P(x|+)}{P(x|-)} = \frac{L(+|x)}{L(-|x)}$$



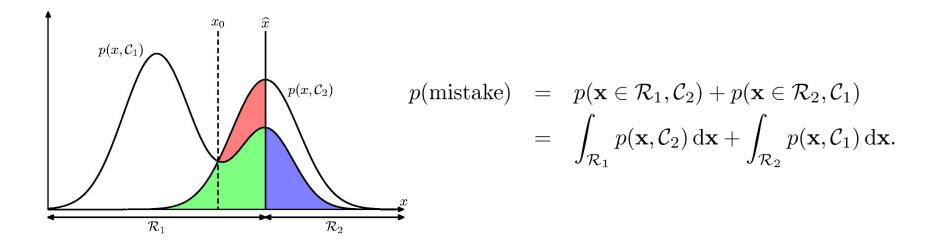
# Very general result. Applies also to multimodal and multivariate distributions.



#### Minimum Misclassification Rate



## Minimum Misclassification Rate



We are free to choose the decision rule that assigns each point x to one of the two classes.

To minimize integrand:  $p(\mathbf{x}, C_k) = p(C_k | \mathbf{x}) p(\mathbf{x})$  must be small Assign x to class for which the posterior  $p(C_k | \mathbf{x})$  is larger!

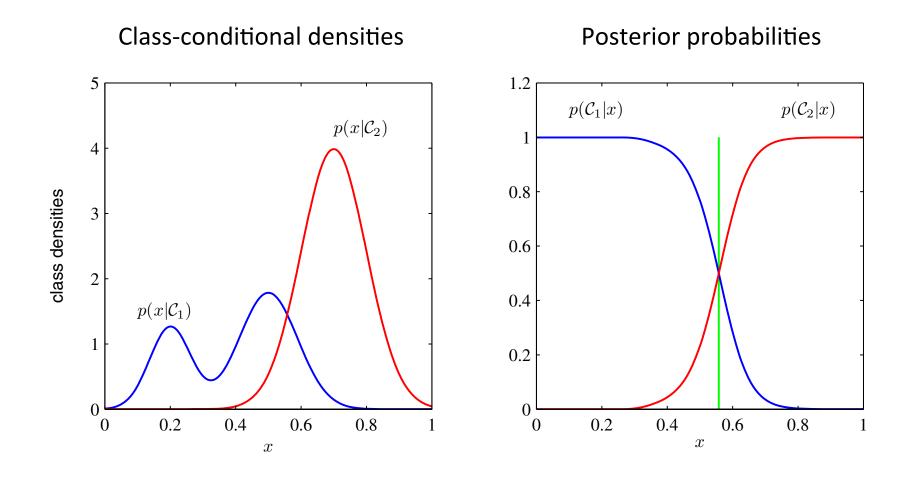
### Three strategies

1. Modeling the class-conditional density for each class  $C_k$ , and prior, then use Bayes

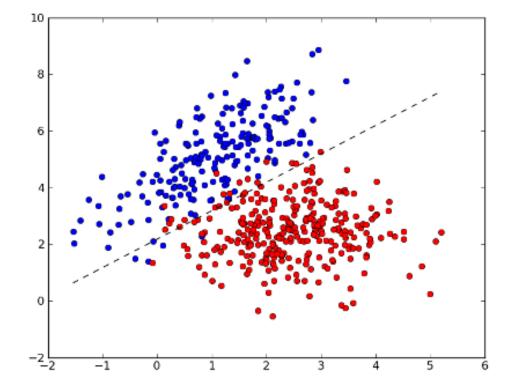
$$p(\mathcal{C}_k | \mathbf{x}) = \frac{p(\mathbf{x} | \mathcal{C}_k) p(\mathcal{C}_k)}{p(\mathbf{x})}$$

- 2. First solve the inference problem of determining the posterior class probabilities  $p(C_k|x)$ , and then subsequently use decision theory to assign each new x to one of the classes
- Find discriminant function that directly maps x to class label

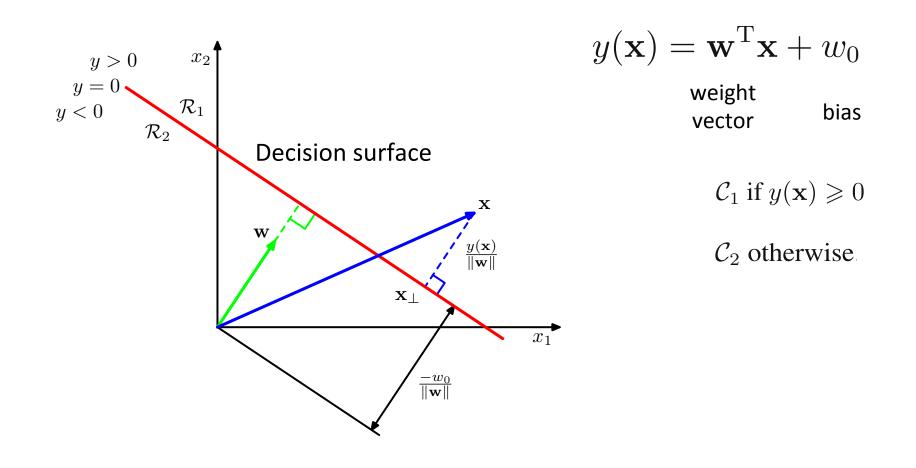
#### Class-conditional density vs. posterior



#### Several dimensions

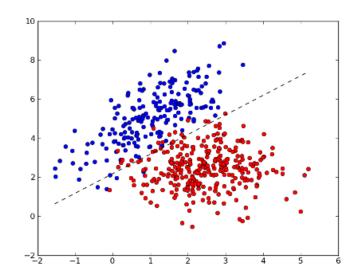


#### Several dimensions



# Projecting data down to one dimension $y = \mathbf{w}^{\mathrm{T}} \mathbf{x}$

But how?



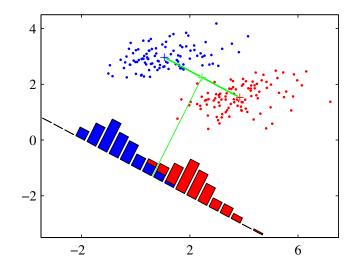
Define class means

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} \mathbf{x}_n,$$

$$\mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} \mathbf{x}_n$$

Try maximize

$$m_2 - m_1 = \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1)$$



# Instead, consider: ratio of between class variance to within class variance

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

With  $s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2$ 

#### Called Fisher criterion. Maximize it!

Maximizing the Fisher Criterion we obtain

$$\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

#### with the total within class covariance

$$\mathbf{S}_{\mathrm{W}} = \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1) (\mathbf{x}_n - \mathbf{m}_1)^{\mathrm{T}} + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2) (\mathbf{x}_n - \mathbf{m}_2)^{\mathrm{T}}$$

#### This is called Fisher's linear discriminant

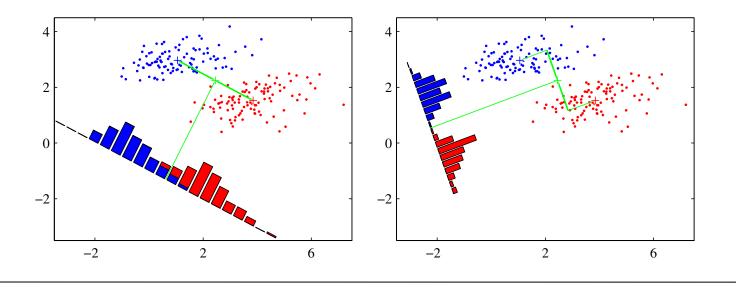
Fisher's linear discriminant

**Fisher Criterion** 

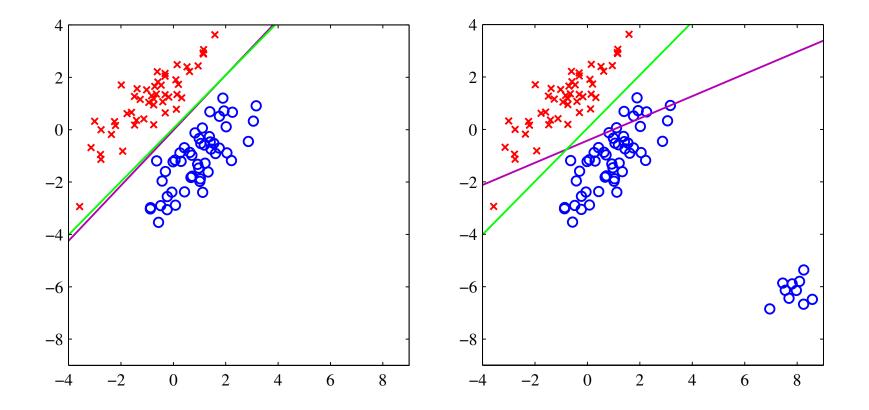
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12

$$\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$
  $J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$ 

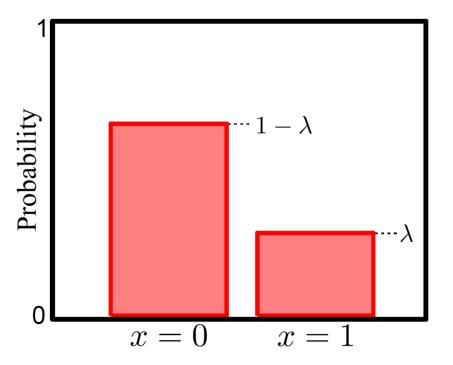


#### Least squares for classification fails



Use logistic regression instead!

## **Bernoulli Distribution**



$$Pr(x = 0) = 1 - \lambda$$
  
 $Pr(x = 1) = \lambda$ .  
or  
 $Pr(x) = \lambda^x (1 - \lambda)^{1-x}$   
For short we write:  
 $Pr(x) = \operatorname{Bern}_x[\lambda]$ 

Bernoulli distribution describes situation where only two possible outcomes y=0/y=1 or failure/success

Takes a single parameter  $\lambda \in [0, 1]$ 

## Logistic Regression

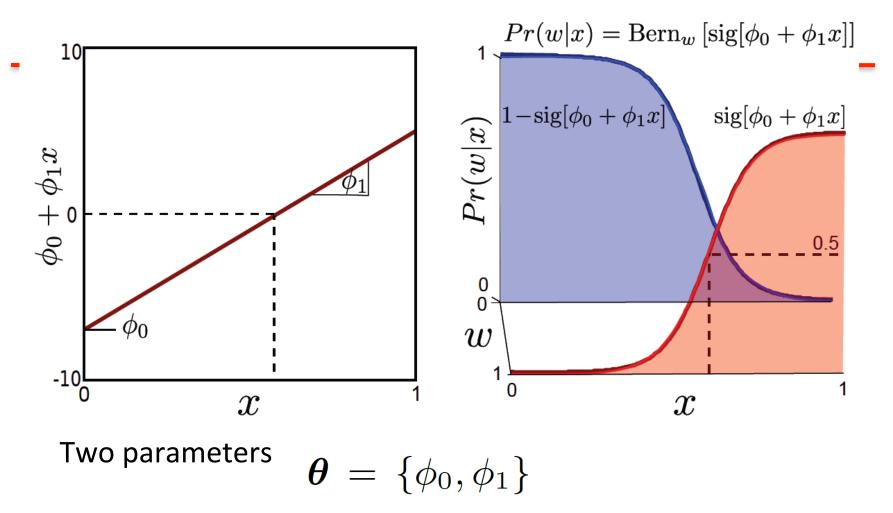
Consider two class problem.

- Choose Bernoulli distribution over world.
- Make parameter  $\lambda$  a function of x

$$Pr(w|\phi_0, \phi, \mathbf{x}) = \operatorname{Bern}_w[\operatorname{sig}[a]]$$

Model activation with a linear function

$$a = \phi_0 + \phi^T \mathbf{x}$$
  
creates number between  $[-\infty, \infty]$ . Maps to  $[0, 1]$  with  
 $\operatorname{sig}[a] = rac{1}{1 + \exp[-a]}$ 



Learning by standard methods (ML,MAP, Bayesian) Inference: Just evaluate Pr(w|x)

## **Neater Notation**

$$Pr(w|\phi_0, \phi, \mathbf{x}) = \operatorname{Bern}_w[\operatorname{sig}[a]]$$

To make notation easier to handle, we

• Attach a 1 to the start of every data vector

$$\mathbf{x}_i \leftarrow \begin{bmatrix} 1 & \mathbf{x}_i^T \end{bmatrix}^T$$

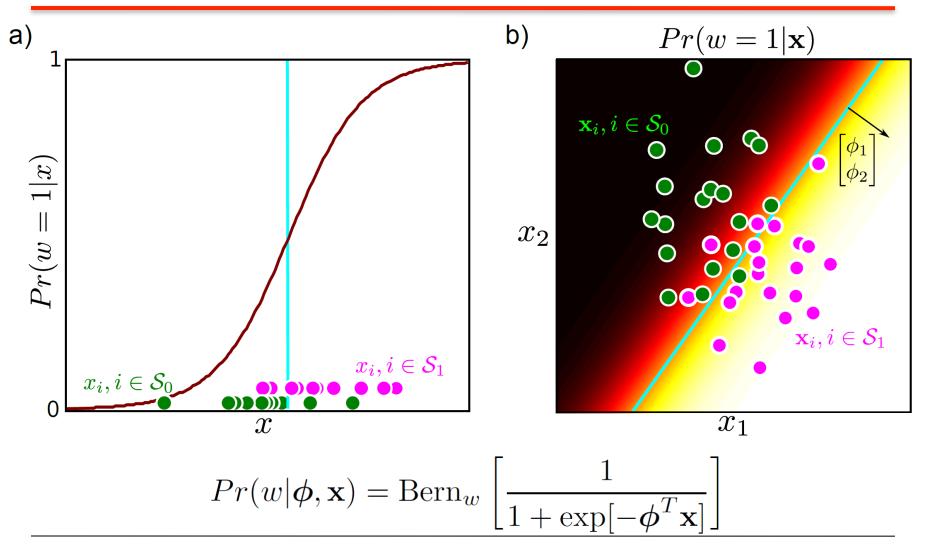
- Attach the offset to the start of the gradient vector  $\boldsymbol{\varphi}$ 

$$\boldsymbol{\phi} \leftarrow [\phi_0 \quad \boldsymbol{\phi}^T]^T$$

New model:

$$Pr(w|\boldsymbol{\phi}, \mathbf{x}) = \operatorname{Bern}_{w} \left[ \frac{1}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}]} \right]$$

## Logistic regression



# Maximum Likelihood

$$Pr(\mathbf{w}|\mathbf{X}, \boldsymbol{\phi}) = \prod_{i=1}^{I} \lambda^{w_i} (1-\lambda)^{1-w_i}$$
$$= \prod_{i=1}^{I} \left( \frac{1}{1+\exp[-\boldsymbol{\phi}^T \mathbf{x}_i]} \right)^{w_i} \left( \frac{\exp[-\boldsymbol{\phi}^T \mathbf{x}_i]}{1+\exp[-\boldsymbol{\phi}^T \mathbf{x}_i]} \right)^{1-w_i}$$

Take logarithm

$$L = \sum_{i=1}^{I} w_i \log \left[ \frac{1}{1 + \exp[-\boldsymbol{\phi}^T \mathbf{x}_i]} \right] + \sum_{i=1}^{I} (1 - w_i) \log \left[ \frac{\exp[-\boldsymbol{\phi}^T \mathbf{x}_i]}{1 + \exp[-\boldsymbol{\phi}^T \mathbf{x}_i]} \right]$$

#### Take derivative:

$$\underline{\frac{\partial L}{\partial \phi}} = -\sum_{i=1}^{I} \left( \frac{1}{1 + \exp[-\phi^T \mathbf{x}_i]} - w_i \right) \mathbf{x}_i = -\sum_{i=1}^{I} \left( \operatorname{sig}[a_i] - w_i \right) \mathbf{x}_i$$

## Derivatives

$$\frac{\partial L}{\partial \boldsymbol{\phi}} = -\sum_{i=1}^{I} \left( \frac{1}{1 + \exp[-\boldsymbol{\phi}^T \mathbf{x}_i]} - w_i \right) \mathbf{x}_i = -\sum_{i=1}^{I} \left( \operatorname{sig}[a_i] - w_i \right) \mathbf{x}_i$$

Unfortunately, there is no closed form solution– we cannot get an expression for  $\phi$  in terms of x and w

Have to use a general purpose technique:

## "iterative non-linear optimization"

## Optimization

Goal:

# $\hat{\boldsymbol{\theta}} = \operatorname*{argmin}_{\boldsymbol{\theta}} [f[\boldsymbol{\theta}]]$

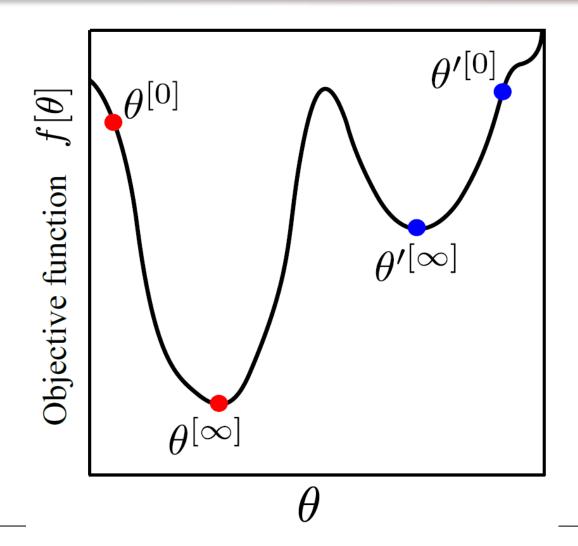
How can we find the minimum?

Cost function or Objective function

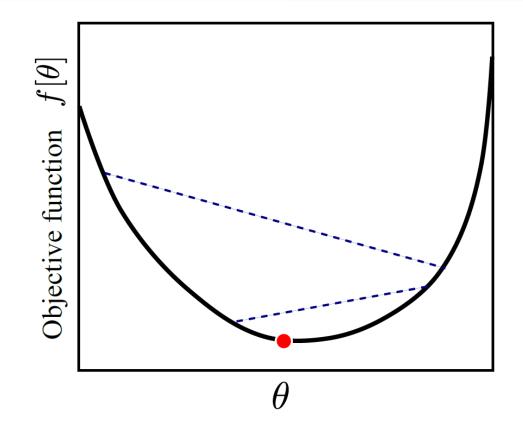
Basic idea:

- Start with estimate  $oldsymbol{ heta}^{[0]}$
- Take a series of small steps to  $oldsymbol{ heta}^{[1]},oldsymbol{ heta}^{[2]}\dotsoldsymbol{ heta}^{[\infty]}$
- Make sure that each step decreases cost
- When can't improve, then must be at minimum

# Local Minima



# Convexity



If a function is convex, then it has only a single minimum. Can tell if a function is convex by looking at 2<sup>nd</sup> derivatives

$$Pr(\mathbf{w}|\mathbf{X}, \boldsymbol{\phi}) = \prod_{i=1}^{I} \left( \frac{1}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]} \right)^{w_{i}} \left( \frac{\exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]} \right)^{1-w_{i}}$$

$$a) Pr(\boldsymbol{\phi}|x_{1...I}, w_{1...I}) \qquad b) \log[Pr(\boldsymbol{\phi}|x_{1...I}, w_{1...I})] \qquad c)$$

$$\phi_{0} \qquad \phi_{0} \qquad f(\boldsymbol{\phi}|x_{1...I}, w_{1...I})] \qquad c)$$

$$L = \sum_{i=1}^{I} w_{i} \log\left[\frac{1}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]}\right] + \sum_{i=1}^{I} (1 - w_{i}) \log\left[\frac{\exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]}\right]$$

Computer vision: models, learning and inference. ©2011 Simon J.D. Prince

## **Gradient Based Optimization**

- Choose a search direction s based on the local properties of the function
- Perform an intensive search along the chosen direction.
   This is called *line search*

$$\hat{\lambda} = \underset{\lambda}{\operatorname{argmin}} \left[ f[\boldsymbol{\theta}^{[t]} + \lambda \mathbf{s}] \right]$$

• Then set

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} + \hat{\lambda} \mathbf{s}$$

## **Gradient Descent**

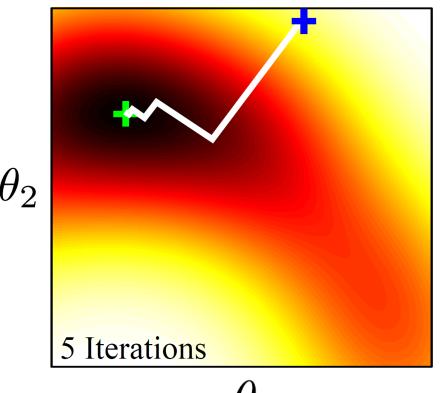
Consider standing on a hillside

Look at gradient where you are standing

Find the steepest direction downhill

Walk in that direction for some distance (line search)

#### Steepest Descent



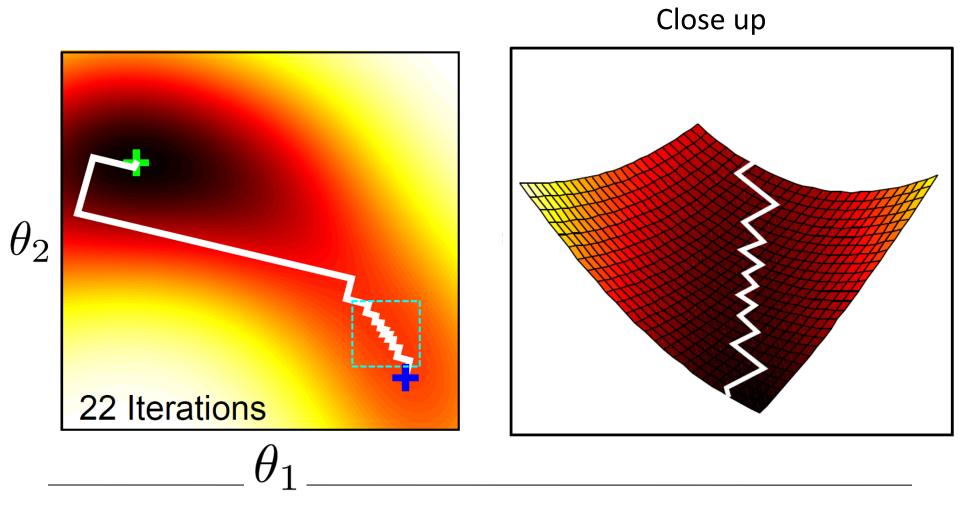
What if we can't compute the gradient?

Compute finite difference approximation:

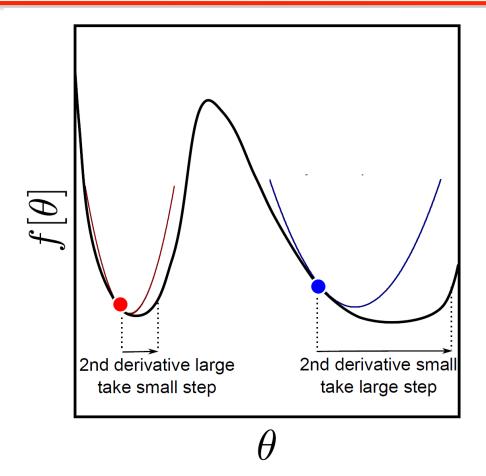
$$\frac{\partial f}{\partial \theta_j} \approx \frac{f \left[ \boldsymbol{\theta} + a \mathbf{e}_j \right] - f \left[ \boldsymbol{\theta} \right]}{a}$$

## where **e**<sub>i</sub> is the unit vector in the j<sup>th</sup> direction

## **Steepest Descent Problems**



## Second Derivatives



In higher dimensions, 2<sup>nd</sup> derivatives change how much we should move in the different directions: changes best direction to move in.

## Newton's Method

Approximate function with Taylor expansion

$$f[\boldsymbol{\theta}] \approx f[\boldsymbol{\theta}^{[t]}] + (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})^T \left. \frac{\partial f}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}^{[t]}} + \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})^T \left. \frac{\partial^2 f}{\partial \boldsymbol{\theta}^2} \right|_{\boldsymbol{\theta}^{[t]}} (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})$$

Take derivative

$$\frac{\partial f}{\partial \boldsymbol{\theta}} \approx \left. \frac{\partial f}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}^{[t]}} + \left. \frac{\partial^2 f}{\partial \boldsymbol{\theta}^2} \right|_{\boldsymbol{\theta}^{[t]}} \left( \boldsymbol{\theta} - \boldsymbol{\theta}^{[t]} \right) = 0$$

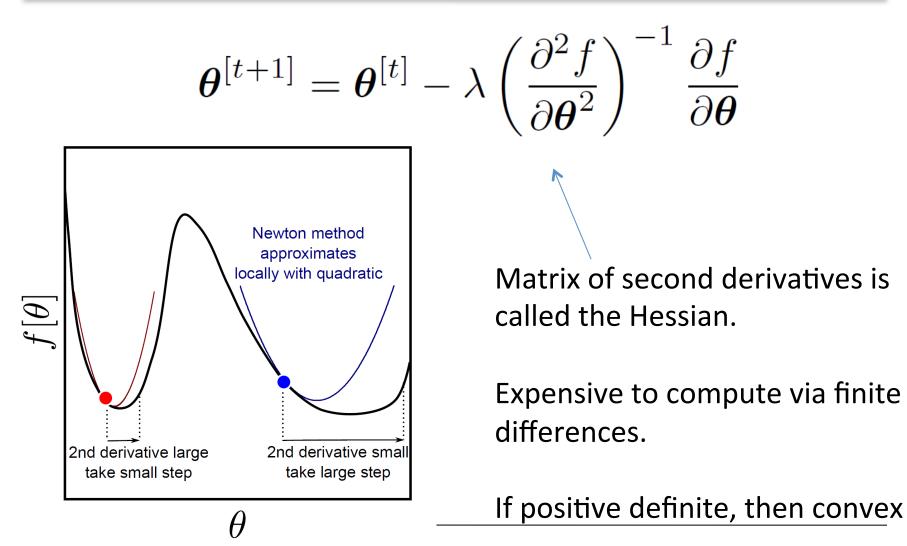
Re-arrange

$$\hat{\boldsymbol{\theta}} = \boldsymbol{\theta}^{[t]} - \left(\frac{\partial^2 f}{\partial \boldsymbol{\theta}^2}\right)^{-1} \frac{\partial f}{\partial \boldsymbol{\theta}}$$
 (derivatives taken at time t)

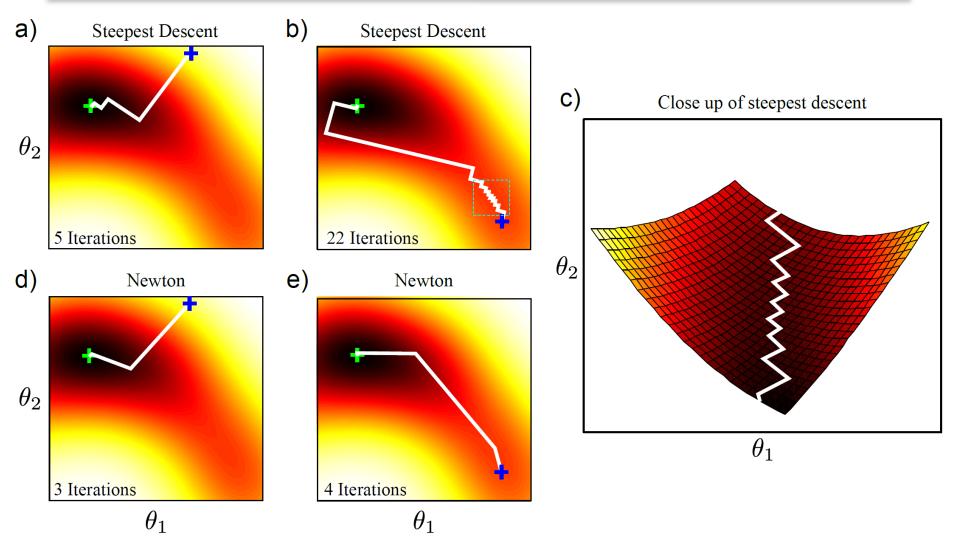
Adding line search

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \lambda \left(\frac{\partial^2 f}{\partial \boldsymbol{\theta}^2}\right)^{-1} \frac{\partial f}{\partial \boldsymbol{\theta}}$$

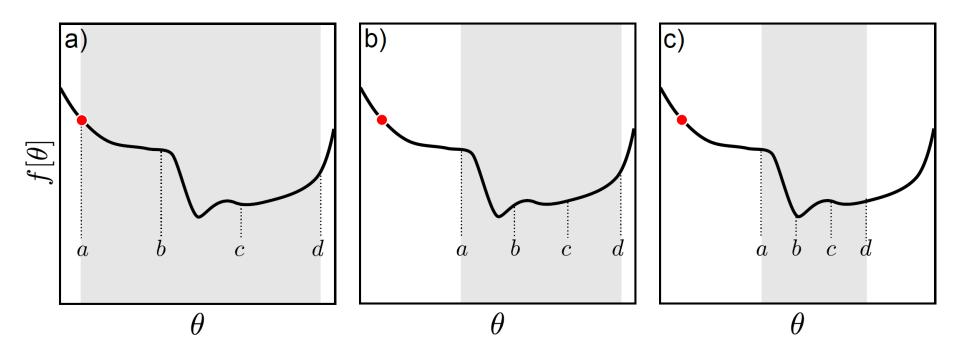
# Newton's Method



## Newton vs. Steepest Descent



## Line Search

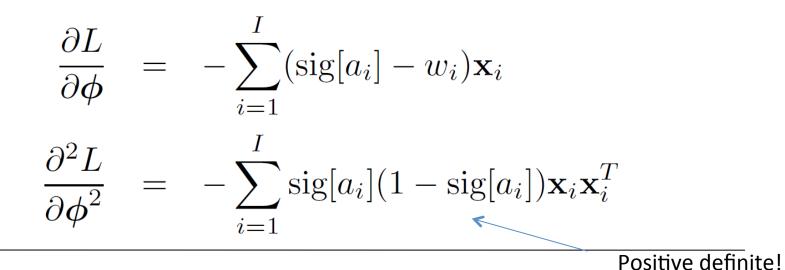


### Gradually narrow down range

## **Optimization for Logistic Regression**

$$\boldsymbol{\phi}^{[t]} = \boldsymbol{\phi}^{[t-1]} + \alpha \left(\frac{\partial^2 L}{\partial \boldsymbol{\phi}^2}\right)^{-1} \frac{\partial L}{\partial \boldsymbol{\phi}}$$

Derivatives of log likelihood:



$$Pr(\mathbf{w}|\mathbf{X}, \boldsymbol{\phi}) = \prod_{i=1}^{I} \left( \frac{1}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]} \right)^{w_{i}} \left( \frac{\exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]}{1 + \exp[-\boldsymbol{\phi}^{T}\mathbf{x}_{i}]} \right)^{1-w_{i}}$$

$$a) Pr(\boldsymbol{\phi}|x_{1...I}, w_{1...I}) \qquad b) \log[Pr(\boldsymbol{\phi}|x_{1...I}, w_{1...I})] \qquad c)$$

$$\phi_{0} \qquad \phi_{0} \qquad \phi_{0} \qquad \phi_{0} \qquad \phi_{0} \qquad \phi_{0} \qquad f(\boldsymbol{\phi}|x_{1...I}, w_{1...I})] \qquad f(\boldsymbol{\phi}|x_{1...I}, w_{1...I}) \qquad f(\boldsymbol{\phi}|x_{1...I}, w_{1..II}) \qquad f(\boldsymbol{\phi}|x_{1..II}, w_{1..II}) \qquad f(\boldsymbol{\phi}|x_{1..II$$

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# Maximum likelihood fits

