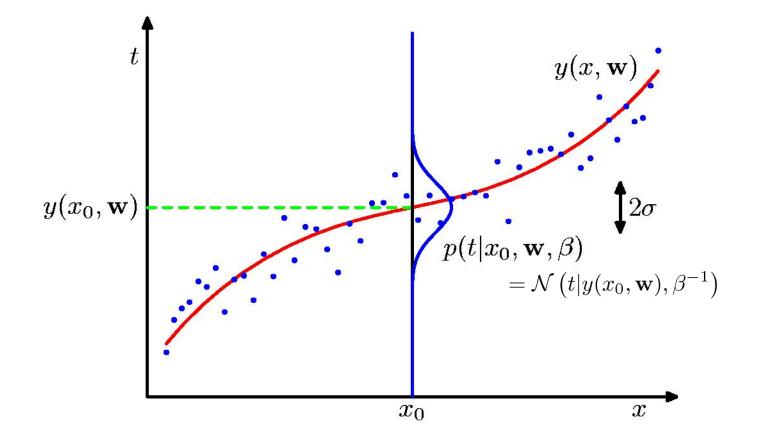
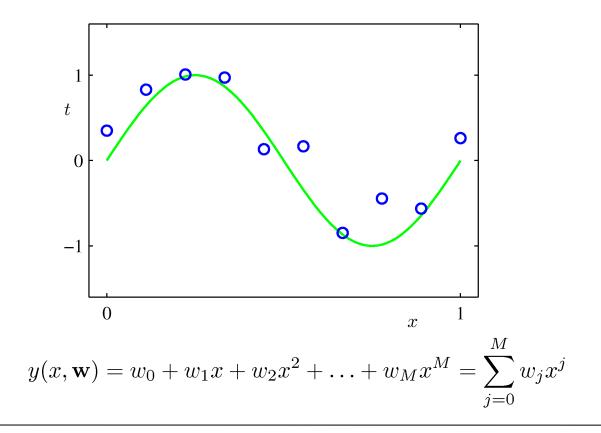
Curve Fitting Re-visited



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 : $\phi_d(x) = x_d$.

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

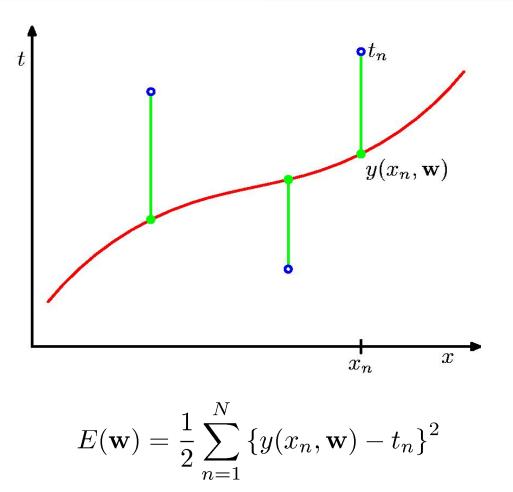
$$\mathbf{Data} \quad \begin{array}{l} \mathbf{x} = (x_1, \dots, x_N)^{\mathrm{T}} \\ \mathbf{t} = (t_1, \dots, t_N)^{\mathrm{T}} \end{array}$$

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

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

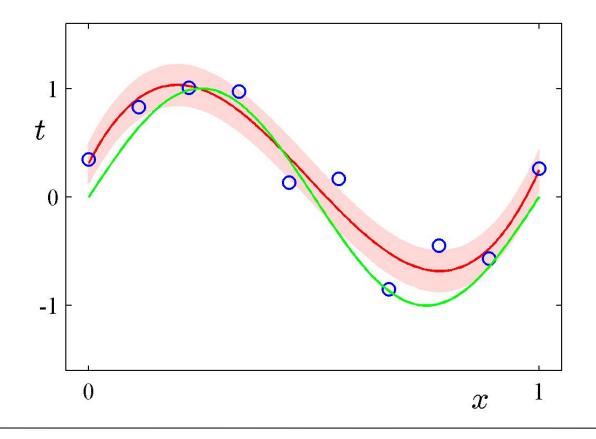
$$\frac{1}{\beta_{\rm ML}} = \frac{1}{N} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}_{\rm ML}) - t_n \}^2$$

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}_{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

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

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

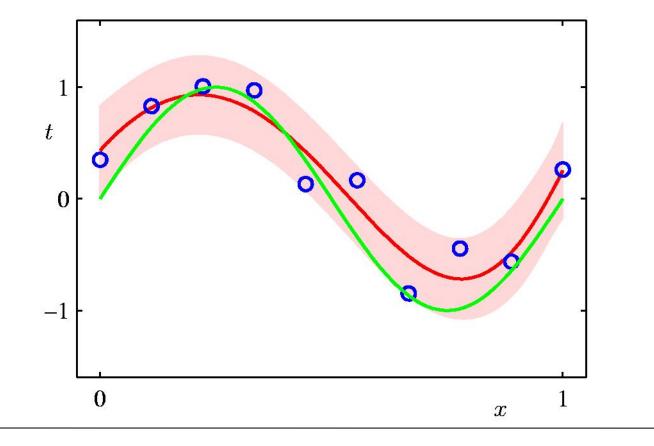
$$m(x) = \beta \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) t_n \qquad s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \boldsymbol{\phi}(x)$$

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 $oldsymbol{\phi}(x_n) = \left(x_n^0, \dots, x_n^M
ight)^{ ext{T}}$

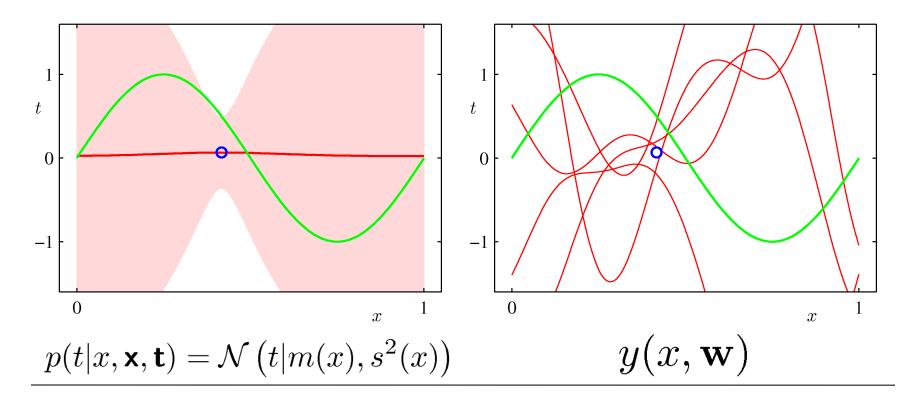
Bayesian Predictive Distribution

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



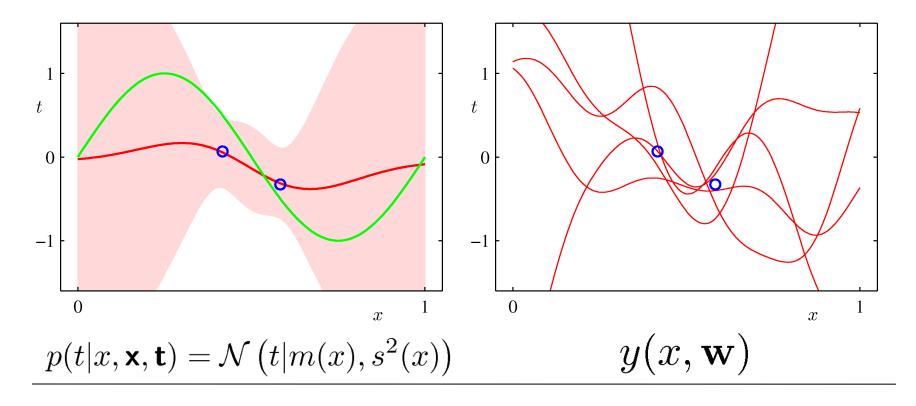
Predictive Distribution (2)

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



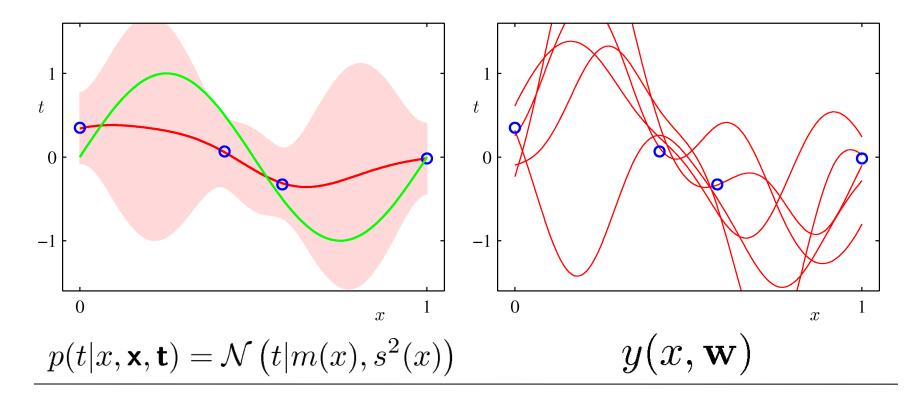
Predictive Distribution (3)

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



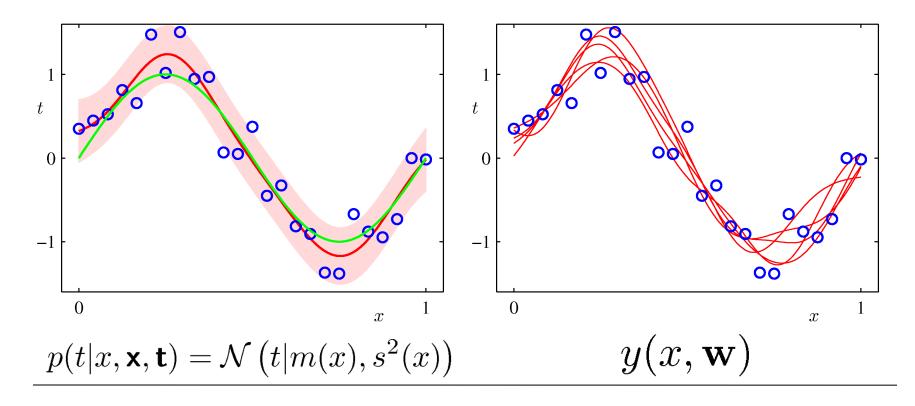
Predictive Distribution (4)

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:

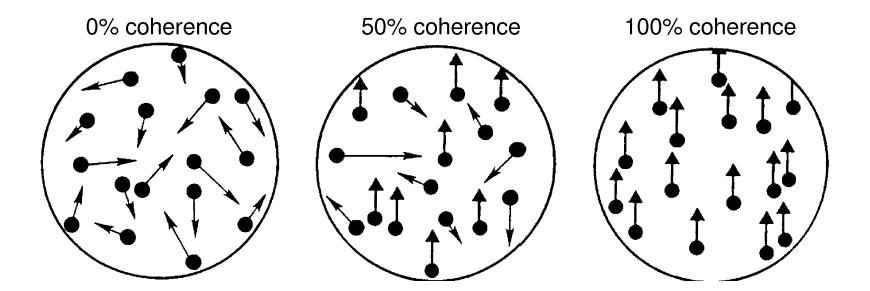
$$x \in [-\infty, \infty], t \in [-\infty, \infty]$$

Classification:

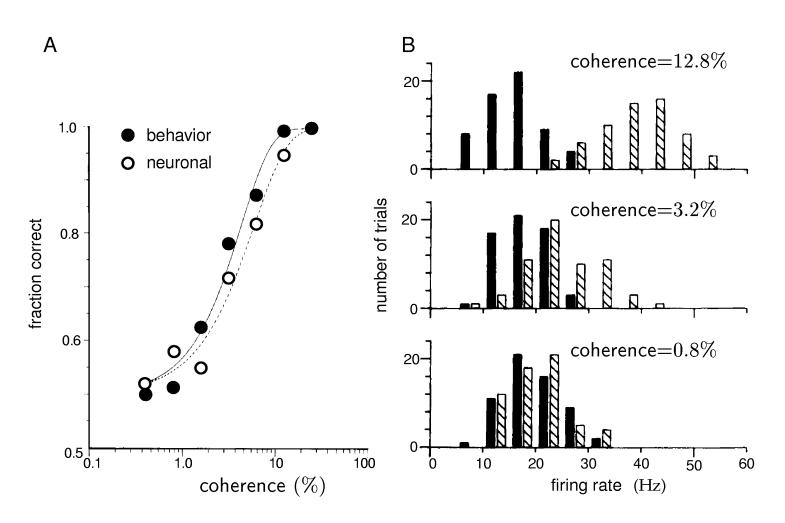
 $x\in [-\infty,\infty], t\in \{0,1\}$

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!

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

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

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

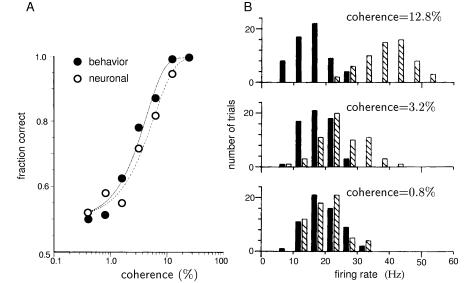
 $P(+) P(x_0|+) = P(-)P(x_0|-)$

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

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

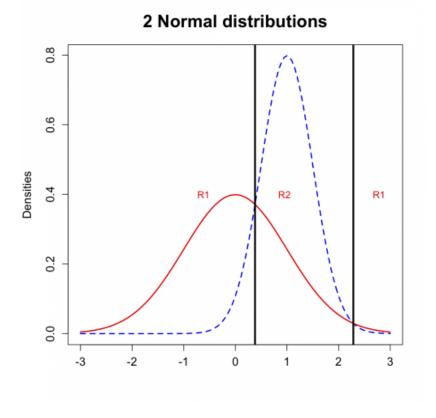
$$P(x_0|+) = P(x_0|-)$$

Set threshold where two probabilities cross



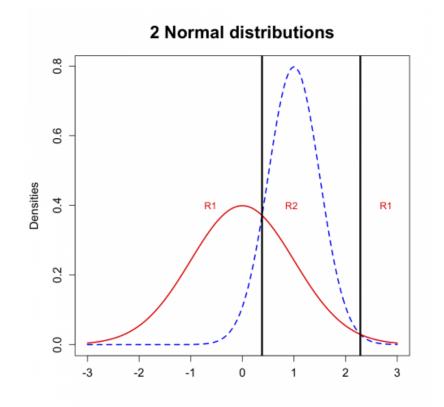
$$P(x_0|+) = P(x_0|-)$$

There can be several dividing lines

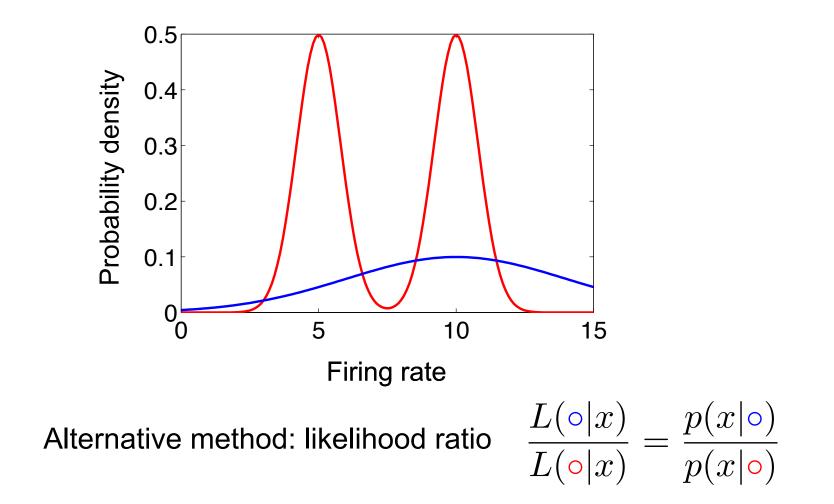


In general: One cannot do better than the likelihood ratio

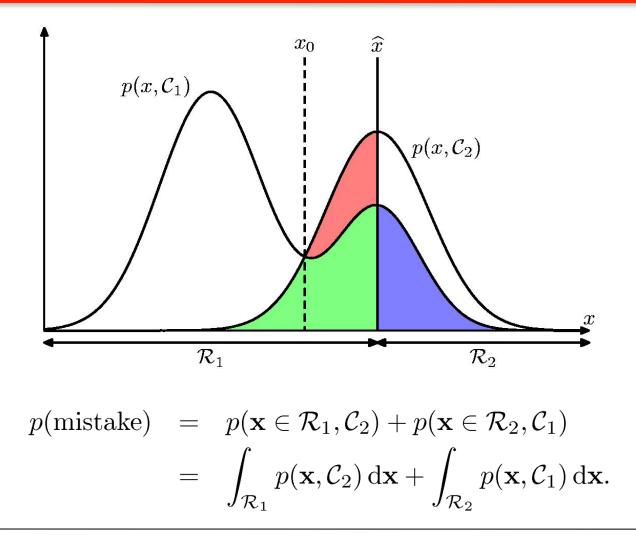
$$l(x) = \frac{P(x|+)}{P(x|-)} = \frac{L(+|x)}{L(-|x)}$$



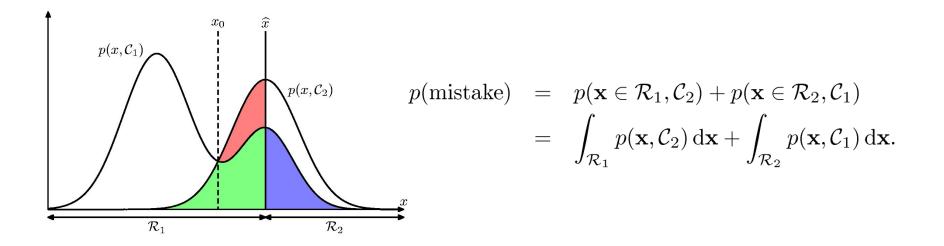
Very general result. Applies also to multimodal and multivariate distributions.



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!

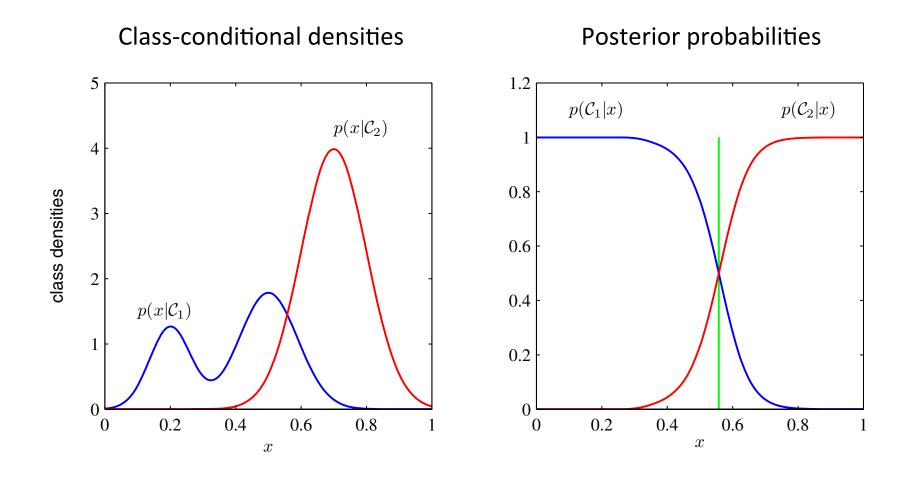
Three strategies

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

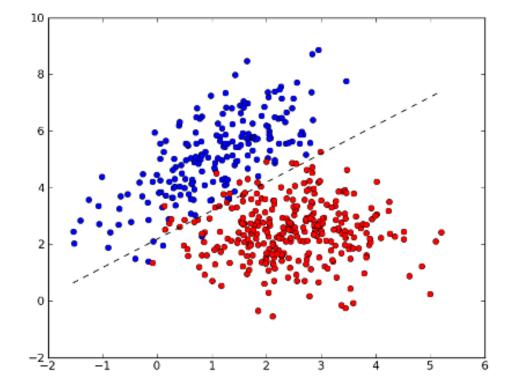
$$p(\mathcal{C}_k | \mathbf{x}) = \frac{p(\mathbf{x} | \mathcal{C}_k) p(\mathcal{C}_k)}{p(\mathbf{x})}$$

- 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

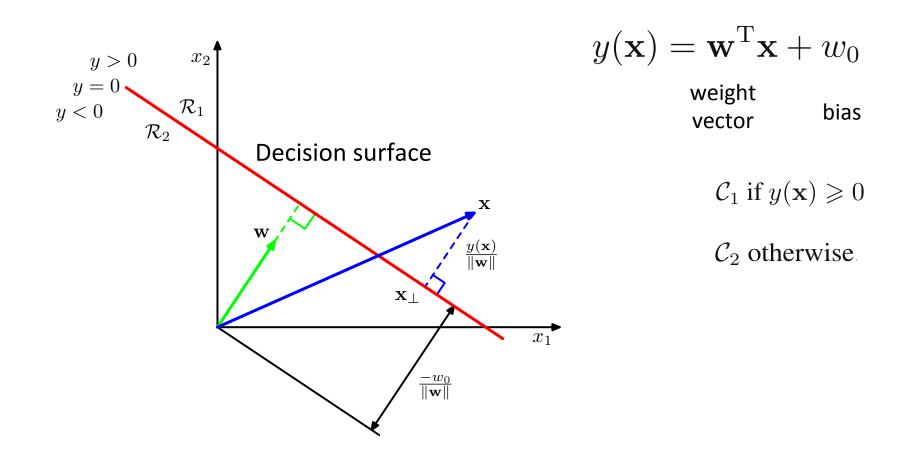
Class-conditional density vs. posterior



Several dimensions

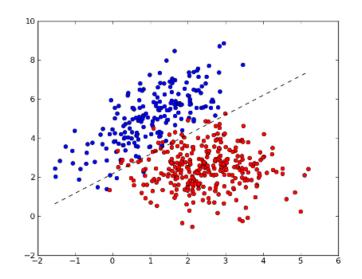


Several dimensions



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

But how?



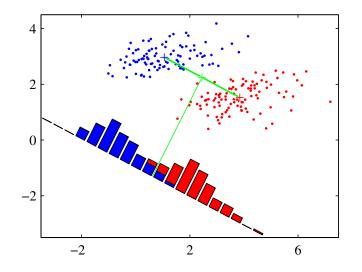
Define class means

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

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

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

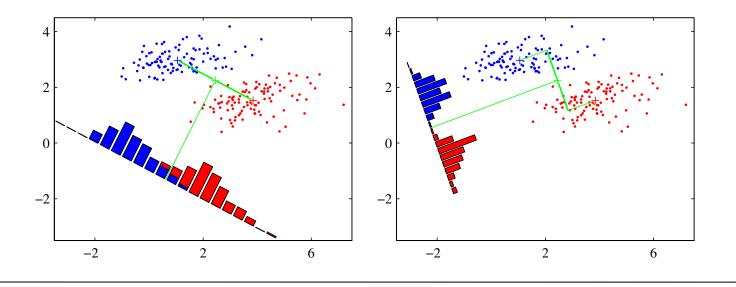
Fisher's linear discriminant

Fisher Criterion

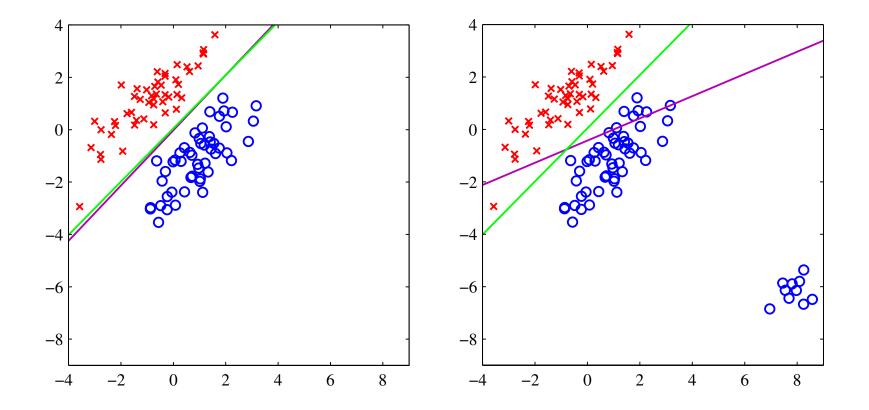
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$$\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$
 $J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$

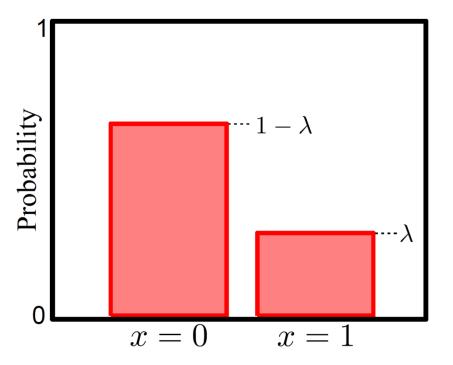


Least squares for classification fails



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.

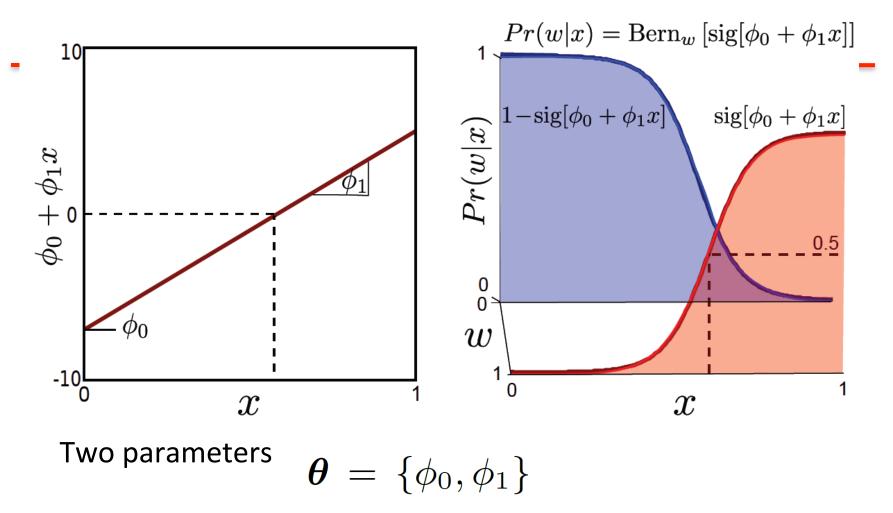
- Choose Bernoulli distribution over world.
- Make parameter λ a function of x

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

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

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

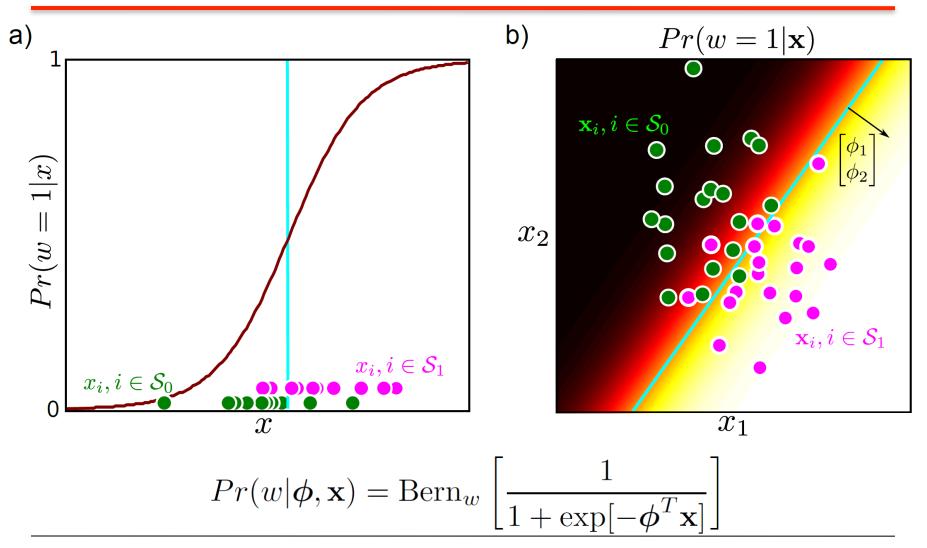
- Attach the offset to the start of the gradient vector $\boldsymbol{\varphi}$

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

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 ϕ in terms of x and w

Have to use a general purpose technique:

"iterative non-linear optimization"

Optimization

Goal:

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

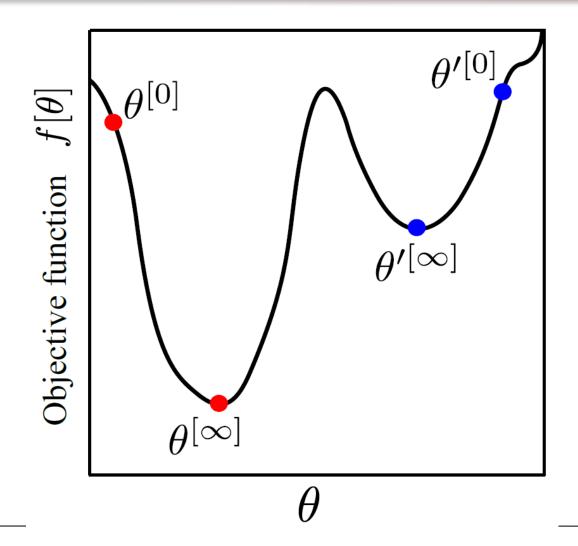
How can we find the minimum?

Cost function or Objective function

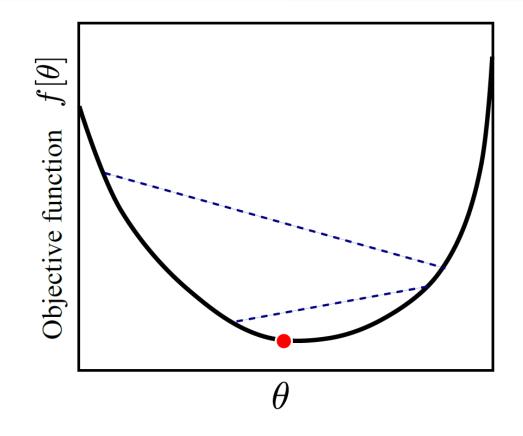
Basic idea:

- 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 2nd derivatives

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

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

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

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

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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

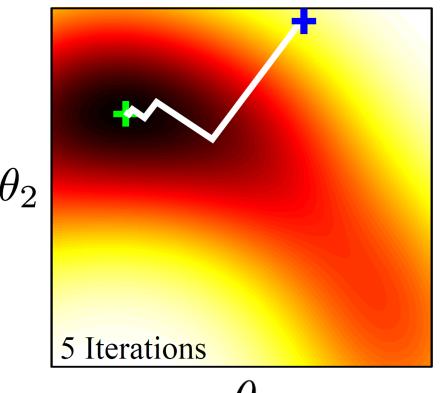
Consider standing on a hillside

Look at gradient where you are standing

Find the steepest direction downhill

Walk in that direction for some distance (line search)

Steepest Descent



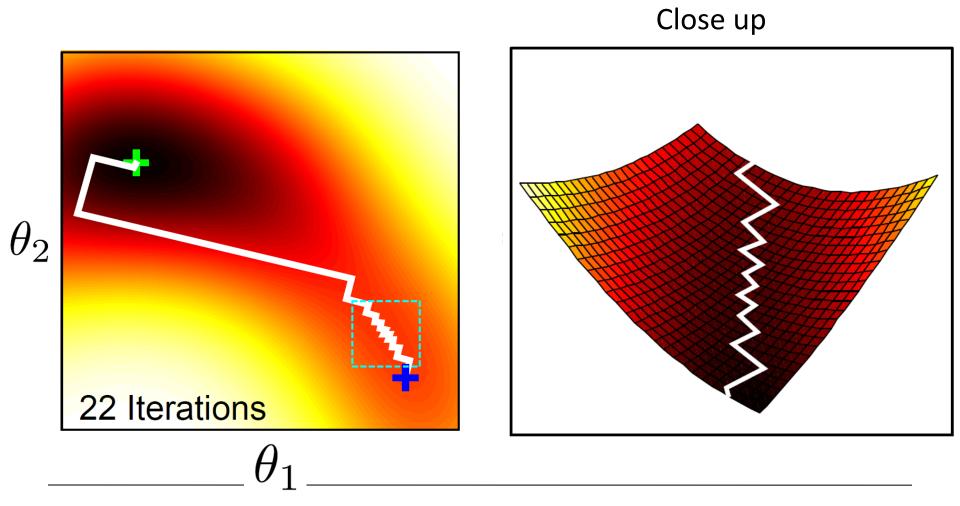
What if we can't compute the gradient?

Compute finite difference approximation:

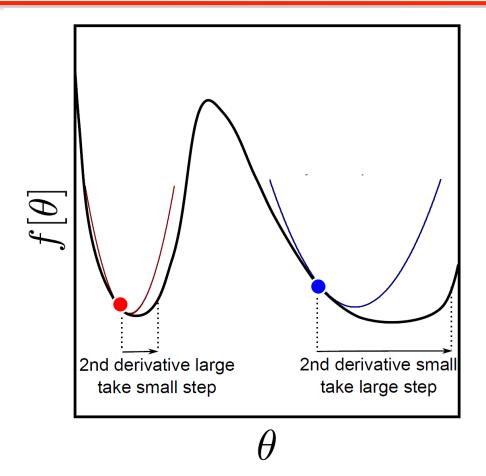
$$\frac{\partial f}{\partial \theta_j} \approx \frac{f \left[\boldsymbol{\theta} + a \mathbf{e}_j \right] - f \left[\boldsymbol{\theta} \right]}{a}$$

where **e**_i is the unit vector in the jth direction

Steepest Descent Problems



Second Derivatives



In higher dimensions, 2nd 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

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

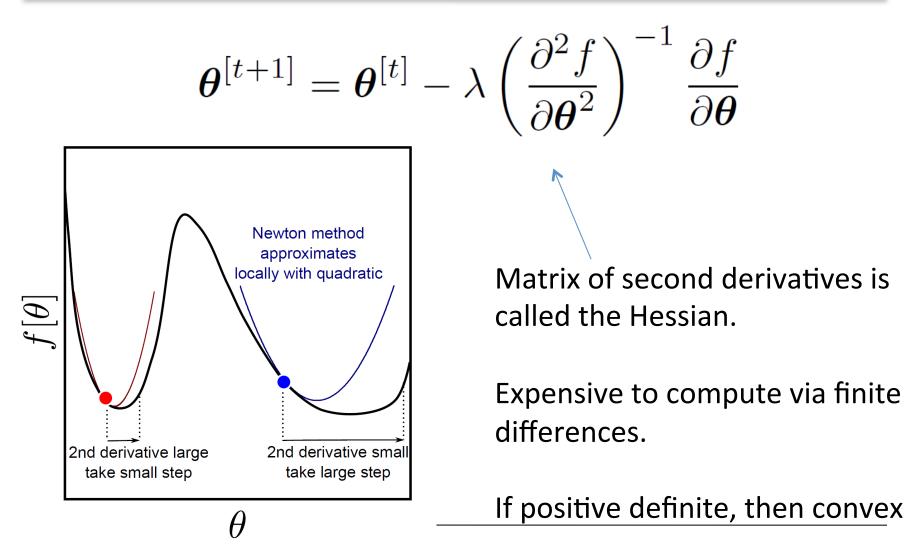
Re-arrange

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

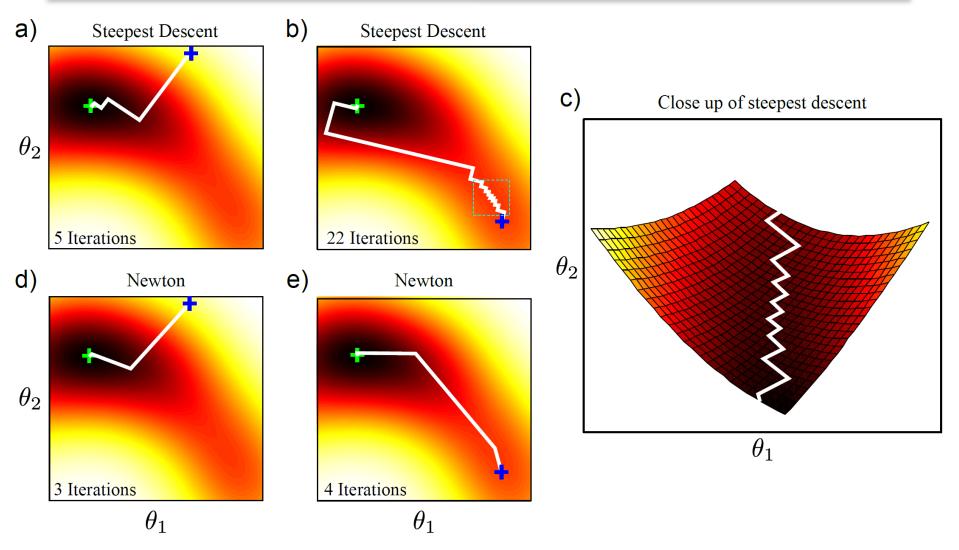
Adding line search

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

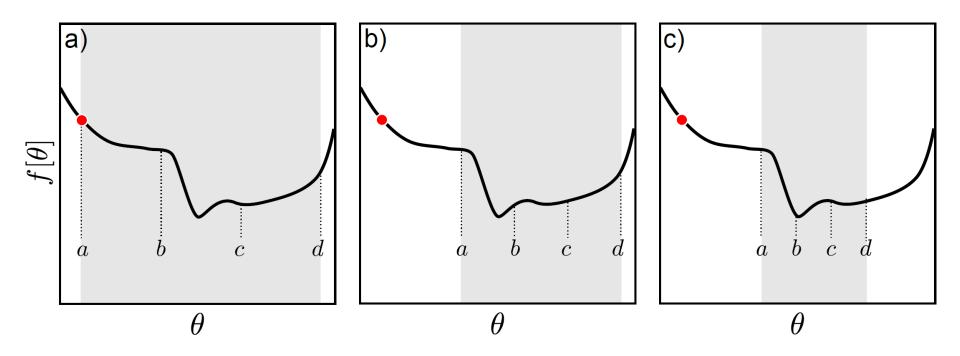
Newton's Method



Newton vs. Steepest Descent



Line Search

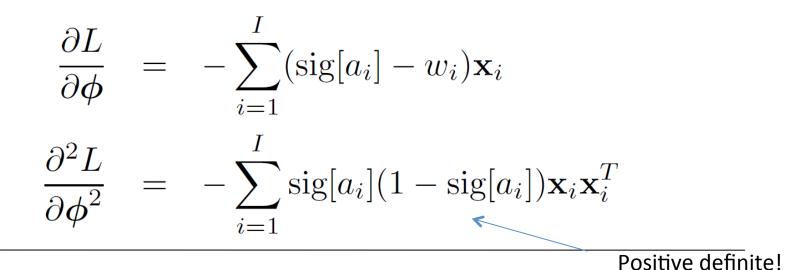


Gradually narrow down range

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

