## Curve Fitting Re-visited



## Linear Basis Function Models (1)

## Example: Polynomial Curve Fitting



$$
y(x, \mathbf{w})=w_{0}+w_{1} x+w_{2} x^{2}+\ldots+w_{M} x^{M}=\sum_{j=0}^{M} w_{j} x^{j}
$$

## 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: $\phi_{d}(x)=X_{d}$.

## Maximum Likelihood

$$
\begin{gathered}
p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta)=\prod_{n=1}^{N} \mathcal{N}\left(t_{n} \mid y\left(x_{n}, \mathbf{w}\right), \beta^{-1}\right) \\
\text { Data } \begin{array}{r}
\mathbf{x}=\left(x_{1}, \ldots, x_{N}\right)^{\mathrm{T}} \\
\mathbf{t}=\left(t_{1}, \ldots, t_{N}\right)^{\mathrm{T}}
\end{array} \\
\ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta)=-\underbrace{\frac{\beta}{2} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}\right)-t_{n}\right\}^{2}}_{\beta E(\mathbf{w})}+\frac{N}{2} \ln \beta-\frac{N}{2} \ln (2 \pi)
\end{gathered}
$$

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

$$
\frac{1}{\beta_{\mathrm{ML}}}=\frac{1}{N} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}_{\mathrm{ML}}\right)-t_{n}\right\}^{2}
$$

## Sum-of-Squares Error Function



## Predictive Distribution

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



## MAP: A Step towards Bayes

$$
\begin{gathered}
p(\mathbf{w} \mid \alpha)=\mathcal{N}\left(\mathbf{w} \mid \mathbf{0}, \alpha^{-1} \mathbf{I}\right)=\left(\frac{\alpha}{2 \pi}\right)^{(M+1) / 2} \exp \left\{-\frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}\right\} \\
p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) p(\mathbf{w} \mid \alpha) \\
\beta \widetilde{E}(\mathbf{w})=\frac{\beta}{2} \sum_{n=1}^{N}\left\{y\left(x_{n}, \mathbf{w}\right)-t_{n}\right\}^{2}+\frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}
\end{gathered}
$$

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

## Bayesian Curve Fitting

$$
\begin{gathered}
p(t \mid x, \mathbf{x}, \mathbf{t})=\int p(t \mid x, \mathbf{w}) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) \mathrm{d} \mathbf{w}=\mathcal{N}\left(t \mid m(x), s^{2}(x)\right) \\
\text { Training data } \quad \begin{array}{r}
\mathbf{x}=\left(x_{1}, \ldots, x_{N}\right)^{\mathrm{T}} \\
\mathbf{t}=\left(t_{1}, \ldots, t_{N}\right)^{\mathrm{T}}
\end{array} \\
m(x)=\beta \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}\left(x_{n}\right) t_{n} \quad s^{2}(x)=\beta^{-1}+\boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \boldsymbol{\phi}(x) \\
\text { Where } \quad \mathbf{S}^{-1}=\alpha \mathbf{I}+\beta \sum_{n=1}^{N} \boldsymbol{\phi}\left(x_{n}\right) \boldsymbol{\phi}\left(x_{n}\right)^{\mathrm{T}}
\end{gathered}
$$

E.g. polynomials as basis functions

$$
\boldsymbol{\phi}\left(x_{n}\right)=\left(x_{n}^{0}, \ldots, x_{n}^{M}\right)^{\mathrm{T}}
$$

## Bayesian Predictive Distribution

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



## Predictive Distribution (2)

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

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

$y(x, \mathbf{w})$

## Predictive Distribution (3)

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

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

$y(x, \mathbf{w})$

## Predictive Distribution (4)

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


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

$y(x, \mathbf{w})$

## Predictive Distribution (5)

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

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

$y(x, \mathbf{w})$

## 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


50\% coherence


100\% coherence


- 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



## Maximum likelihood

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

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

Intuition: Divide x axis at critical point $\mathrm{x}_{0}$ : Everything to right is called a +, everything to the left a -

How should we choose $x_{0}$ ?

## Maximum likelihood

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 + :

$$
P(\text { say }+\mid \text { signal is }+)=\int_{x_{0}}^{\infty} d x P(x \mid+)
$$

Probability of correctly identifying signal -:

$$
P(\text { say }-\mid \text { signal is }-)=\int_{\infty}^{x_{0}} d x P(x \mid-)
$$

Probability of making correct choice:

$$
P_{c}\left(x_{0}\right)=P(+) \int_{x_{0}}^{\infty} d x P(x \mid+)+P(-) \int_{\infty}^{x_{0}} d x P(x \mid-)
$$

## Maximum likelihood

Probability of making correct choice:

$$
P_{c}\left(x_{0}\right)=P(+) \int_{x_{0}}^{\infty} d x P(x \mid+)+P(-) \int_{\infty}^{x_{0}} d x P(x \mid-)
$$

Maximize it!

$$
\frac{d P_{c}\left(x_{0}\right)}{d x_{0}}=0
$$

$$
\begin{gathered}
P(+) \frac{d}{d x_{0}} \int_{x_{0}}^{\infty} d x P(x \mid+)+P(-) \frac{d}{d x_{0}} \int_{\infty}^{x_{0}} d x P(x \mid-)=0 \\
-P(+) P\left(x_{0} \mid+\right)+P(-) P\left(x_{0} \mid-\right)=0 \\
P(+) P\left(x_{0} \mid+\right)=P(-) P\left(x_{0} \mid-\right)
\end{gathered}
$$

## Maximum likelihood

$$
P(+) P\left(x_{0} \mid+\right)=P(-) P\left(x_{0} \mid-\right)
$$

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

$$
P\left(x_{0} \mid+\right)=P\left(x_{0} \mid-\right)
$$

Set threshold where two probabilities cross


## Maximum likelihood

$$
\rightleftarrows P\left(x_{0} \mid+\right)=P\left(x_{0} \mid-\right)
$$

There can be several dividing lines


## Maximum likelihood

In general: One cannot do better than the likelihood ratio

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

2 Normal distributions


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


Firing rate
Alternative method: likelihood ratio $\frac{L(\circ \mid x)}{L(\circ \mid x)}=\frac{p(x \mid \circ)}{p(x \mid \circ)}$

## Minimum Misclassification Rate

$$
\begin{aligned}
& p(\text { mistake })=p\left(\mathbf{x} \in \mathcal{R}_{1}, \mathcal{C}_{2}\right)+p\left(\mathbf{x} \in \mathcal{R}_{2}, \mathcal{C}_{1}\right) \\
& =\int_{\mathcal{R}_{1}} p\left(\mathbf{x}, \mathcal{C}_{2}\right) \mathrm{d} \mathbf{x}+\int_{\mathcal{R}_{2}} p\left(\mathbf{x}, \mathcal{C}_{1}\right) \mathrm{d} \mathbf{x} .
\end{aligned}
$$

## Minimum Misclassification Rate



$$
\begin{aligned}
p(\text { mistake }) & =p\left(\mathbf{x} \in \mathcal{R}_{1}, \mathcal{C}_{2}\right)+p\left(\mathbf{x} \in \mathcal{R}_{2}, \mathcal{C}_{1}\right) \\
& =\int_{\mathcal{R}_{1}} p\left(\mathbf{x}, \mathcal{C}_{2}\right) \mathrm{d} \mathbf{x}+\int_{\mathcal{R}_{2}} p\left(\mathbf{x}, \mathcal{C}_{1}\right) \mathrm{d} \mathbf{x}
\end{aligned}
$$

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

To minimize integrand: $p\left(\mathbf{x}, \mathcal{C}_{k}\right)=p\left(\mathcal{C}_{k} \mid \mathbf{x}\right) p(\mathbf{x})$ must be small Assign x to class for which the posterior $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$ is larger!

## Three strategies

1. Modeling the class-conditional density for each class $C_{k}$, and prior, then use Bayes

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{p(\mathbf{x})}
$$

2. First solve the inference problem of determining the posterior class probabilities $p\left(C_{k} \mid x\right)$, and then subsequently use decision theory to assign each new $x$ to one of the classes
3. Find discriminant function that directly maps $x$ to class label

## Class-conditional density vs. posterior

Class-conditional densities


Posterior probabilities


## Several dimensions



## Several dimensions



$$
\begin{array}{r}
y(\mathbf{x})=\mathbf{w}^{\mathrm{T}} \mathbf{x}+w_{0} \\
\text { weight } \\
\text { vector } \\
\mathcal{C}_{1} \text { if } y(\mathbf{x}) \geqslant 0 \\
\mathcal{C}_{2} \text { otherwise }
\end{array}
$$

## Fisher's linear discriminant 1

Projecting data down to one dimension

$$
y=\mathbf{w}^{\mathrm{T}} \mathbf{x}
$$

But how?


## Fisher's linear discriminant 2

Define class means

$$
\mathbf{m}_{1}=\frac{1}{N_{1}} \sum_{n \in \mathcal{C}_{1}} \mathbf{x}_{n}, \quad \mathbf{m}_{2}=\frac{1}{N_{2}} \sum_{n \in \mathcal{C}_{2}} \mathbf{x}_{n}
$$

Try maximize

$$
m_{2}-m_{1}=\mathbf{w}^{\mathrm{T}}\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right)
$$



## Fisher's linear discriminant 3

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

$$
J(\mathbf{w})=\frac{\left(m_{2}-m_{1}\right)^{2}}{s_{1}^{2}+s_{2}^{2}}
$$

With

$$
s_{k}^{2}=\sum_{n \in \mathcal{C}_{k}}\left(y_{n}-m_{k}\right)^{2}
$$

Called Fisher criterion. Maximize it!

## Fisher's linear discriminant 4

Maximizing the Fisher Criterion we obtain

$$
\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right)
$$

with the total within class covariance

$$
\mathbf{S}_{\mathrm{W}}=\sum_{n \in \mathcal{C}_{1}}\left(\mathbf{x}_{n}-\mathbf{m}_{1}\right)\left(\mathbf{x}_{n}-\mathbf{m}_{1}\right)^{\mathrm{T}}+\sum_{n \in \mathcal{C}_{2}}\left(\mathbf{x}_{n}-\mathbf{m}_{2}\right)\left(\mathbf{x}_{n}-\mathbf{m}_{2}\right)^{\mathrm{T}}
$$

This is called Fisher's linear discriminant

## Fisher's linear discriminant 4

Fisher's linear discriminant

$$
\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right) \quad J(\mathbf{w})=\frac{\left(m_{2}-m_{1}\right)^{2}}{s_{1}^{2}+s_{2}^{2}}
$$

Fisher Criterion



## Least squares for classification fails




Use logistic regression instead!

## Bernoulli Distribution



$$
\begin{aligned}
& \operatorname{Pr}(x=0)=1-\lambda \\
& \operatorname{Pr}(x=1)=\lambda . \\
& \text { or } \\
& \operatorname{Pr}(x)=\lambda^{x}(1-\lambda)^{1-x} \\
& \text { For short we write: } \\
& \operatorname{Pr}(x)=\operatorname{Bern}_{x}[\lambda]
\end{aligned}
$$

Bernoulli distribution describes situation where only two possible outcomes $\mathrm{y}=0 / \mathrm{y}=1$ 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 $x$

$$
\operatorname{Pr}\left(w \mid \phi_{0}, \boldsymbol{\phi}, \mathbf{x}\right)=\operatorname{Bern}_{w}[\operatorname{sig}[a]]
$$

Model activation with a linear function

$$
a=\phi_{0}+\boldsymbol{\phi}^{T} \mathbf{x}
$$

creates number between $[-\infty, \infty]$. Maps to $[0,1]$ with

$$
\operatorname{sig}[a]=\frac{1}{1+\exp [-a]}
$$




Two parameters

$$
\boldsymbol{\theta}=\left\{\phi_{0}, \phi_{1}\right\}
$$

Learning by standard methods (ML,MAP, Bayesian) Inference: Just evaluate $\operatorname{Pr}(w \mid x)$

## Neater Notation

$$
\operatorname{Pr}\left(w \mid \phi_{0}, \boldsymbol{\phi}, \mathbf{x}\right)=\operatorname{Bern}_{w}[\operatorname{sig}[a]]
$$

To make notation easier to handle, we

- Attach a 1 to the start of every data vector

$$
\mathbf{x}_{i} \leftarrow\left[\begin{array}{ll}
1 & \mathbf{x}_{i}^{T}
\end{array}\right]^{T}
$$

- Attach the offset to the start of the gradient vector $\phi$

$$
\boldsymbol{\phi} \leftarrow\left[\begin{array}{ll}
\phi_{0} & \boldsymbol{\phi}^{T}
\end{array}\right]^{T}
$$

New model:

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

## Logistic regression



## Maximum Likelihood

$$
\begin{aligned}
\operatorname{Pr}(\mathbf{w} \mid \mathbf{X}, \boldsymbol{\phi}) & =\prod_{i=1}^{I} \lambda^{w_{i}}(1-\lambda)^{1-w_{i}} \\
& =\prod_{i=1}^{I}\left(\frac{1}{1+\exp \left[-\boldsymbol{\phi}^{T} \mathbf{x}_{i}\right]}\right)^{w_{i}}\left(\frac{\exp \left[-\phi^{T} \mathbf{x}_{i}\right]}{1+\exp \left[-\phi^{T} \mathbf{x}_{i}\right]}\right)^{1-w_{i}}
\end{aligned}
$$

Take logarithm

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

Take derivative:

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

## Derivatives

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

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:

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

How can we find the minimum?

Basic idea:

Cost function or
Objective function

- Start with estimate $\boldsymbol{\theta}^{[0]}$
- Take a series of small steps to $\boldsymbol{\theta}^{[1]}, \boldsymbol{\theta}^{[2]} \ldots \boldsymbol{\theta}^{[\infty]}$
- 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 $2^{\text {nd }}$ derivatives

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


b) $\quad \log \left[\operatorname{Pr}\left(\phi \mid x_{1 \ldots I}, w_{1 \ldots I}\right)\right]$
c)

$\phi_{0}$

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

## 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

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

- 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


$\theta_{1}$

## Finite differences

What if we can't compute the gradient?

Compute finite difference approximation:

$$
\frac{\partial f}{\partial \theta_{j}} \approx \frac{f\left[\boldsymbol{\theta}+a \mathbf{e}_{j}\right]-f[\boldsymbol{\theta}]}{a}
$$

where $\mathbf{e}_{j}$ is the unit vector in the $j^{\text {th }}$ direction

## Steepest Descent Problems

## Close up


$\theta_{1}$

## Second Derivatives



In higher dimensions, $2^{\text {nd }}$ 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

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

Take derivative

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

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

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


$\theta$

Matrix of second derivatives is called the Hessian.

Expensive to compute via finite differences.

If positive definite, then convex

## Newton vs. Steepest Descent



## Line Search


$\theta$

$\theta$


## Gradually narrow down range

## Optimization for Logistic Regression

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

Derivatives of log likelihood:

$$
\begin{aligned}
\frac{\partial L}{\partial \phi} & =-\sum_{i=1}^{I}\left(\operatorname{sig}\left[a_{i}\right]-w_{i}\right) \mathbf{x}_{i} \\
\frac{\partial^{2} L}{\partial \phi^{2}} & =-\sum_{i=1}^{I} \operatorname{sig}\left[a_{i}\right]\left(1-\operatorname{sig}\left[a_{i}\right]\right) \mathbf{x}_{i} \mathbf{x}_{i}^{T}
\end{aligned}
$$

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


b) $\quad \log \left[\operatorname{Pr}\left(\phi \mid x_{1 \ldots I}, w_{1 \ldots I}\right)\right]$

c)

$\phi_{0}$
$L=\sum_{i=1}^{I} w_{i} \log \left[\frac{1}{1+\exp \left[-\boldsymbol{\phi}^{T} \mathbf{x}_{i}\right]}\right]+\sum_{i=1}^{I}\left(1-w_{i}\right) \log \left[\frac{\exp \left[-\boldsymbol{\phi}^{T} \mathbf{x}_{i}\right]}{1+\exp \left[-\boldsymbol{\phi}^{T} \mathbf{x}_{i}\right]}\right]$

## Maximum likelihood fits

a)


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

