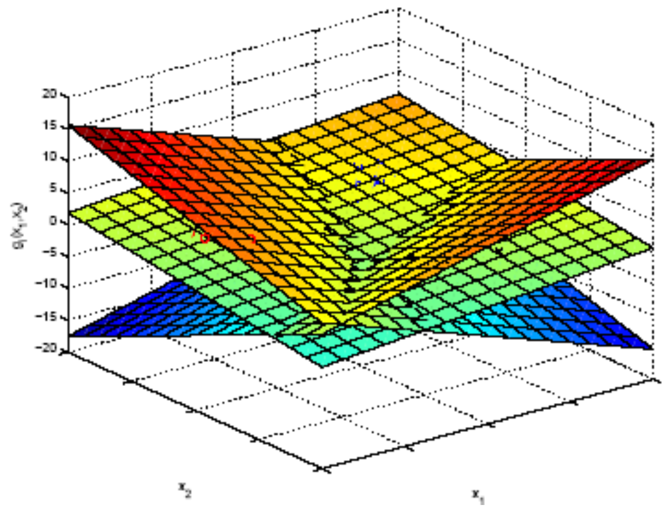
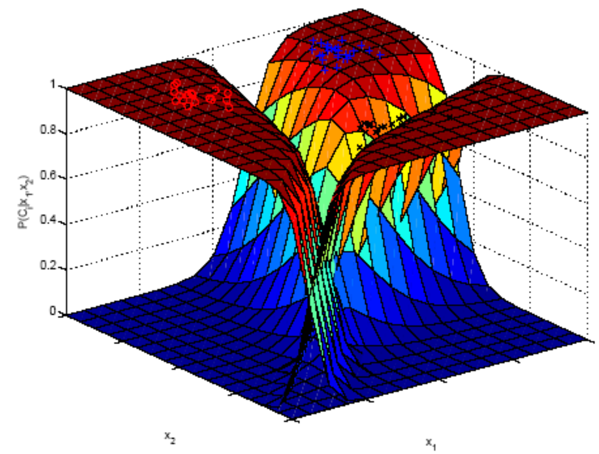
Introduction to Machine Learning





Week 2: Logistic Regression

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Week 1: Machine Learning variants

- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised/semi-supervised

  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: sparse reward for a sequence of decisions

What we want to learn: a function

method

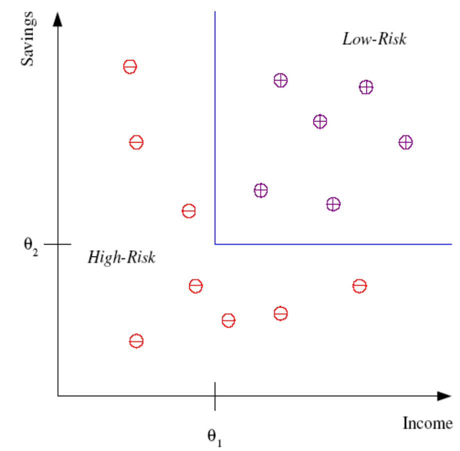
prediction

$$y = f_w(x)$$

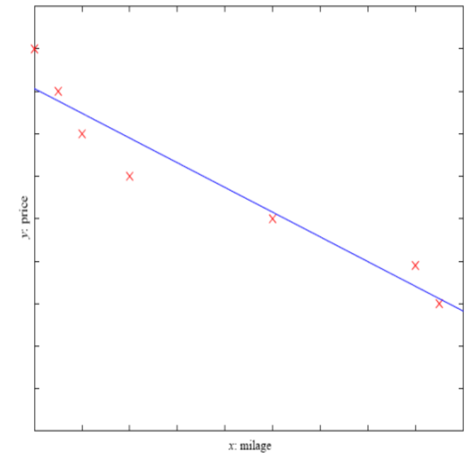
parameters

Input

Classification: $y \in \{0,1\}$



Regression: $y \in \mathbb{R}$



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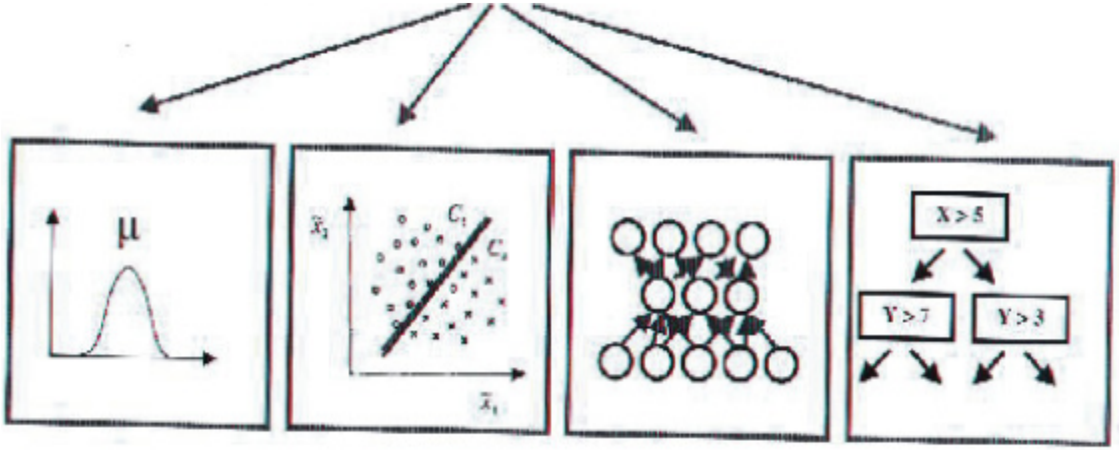


Week 1-4: linear models

$$y = f_{\mathbf{w}}(\mathbf{x}) = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x}$$

Linear classifiers, neural networks, decision trees, ensemble models, probabilistic classifiers, …

What we want to learn: a function

method

prediction

$$y = f_w(x) = f(x; w)$$

parameters

Input

Sum-of-squared errors loss:

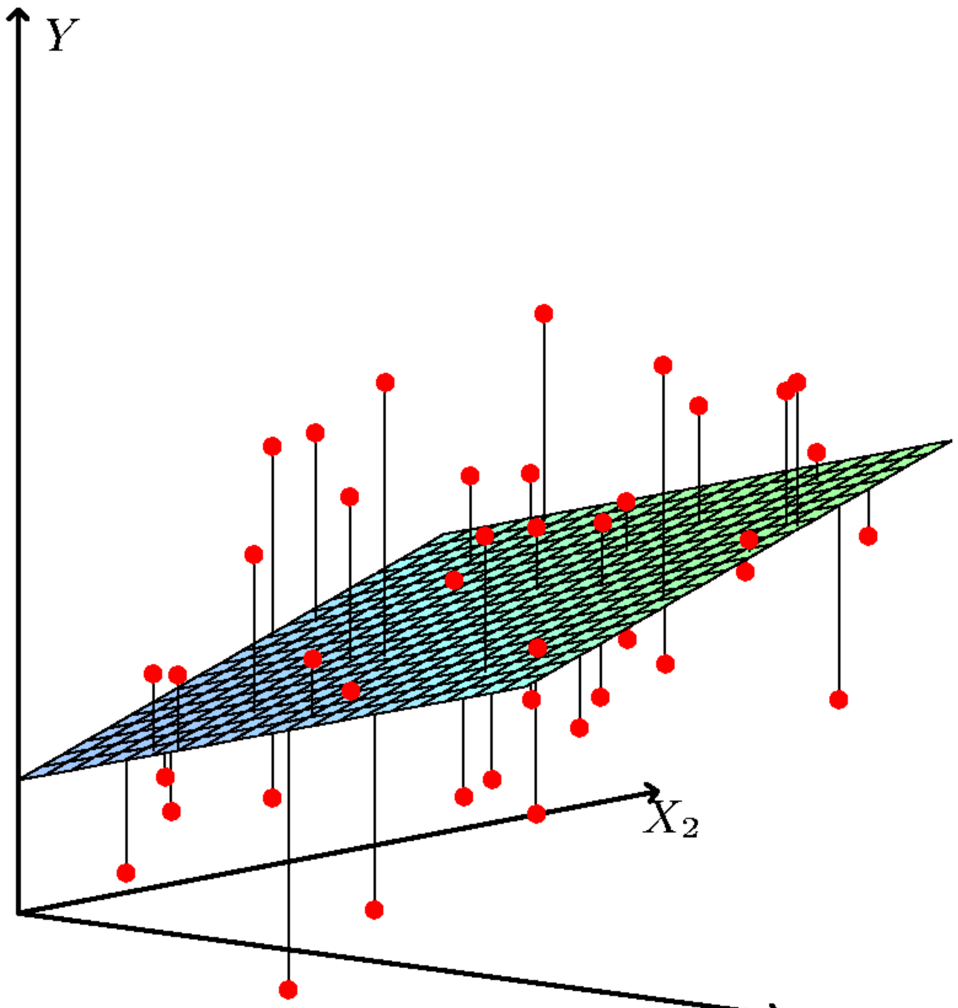
$$L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle)^2$$

$$\mathbf{y} = \begin{bmatrix} y^1 \\ \vdots \\ y^N \end{bmatrix} \mathbf{X} = \begin{bmatrix} (\mathbf{x}^1)^T \\ \hline (\mathbf{x}^2)^T \\ \hline \vdots \\ \hline (\mathbf{x}^N)^T \end{bmatrix}$$

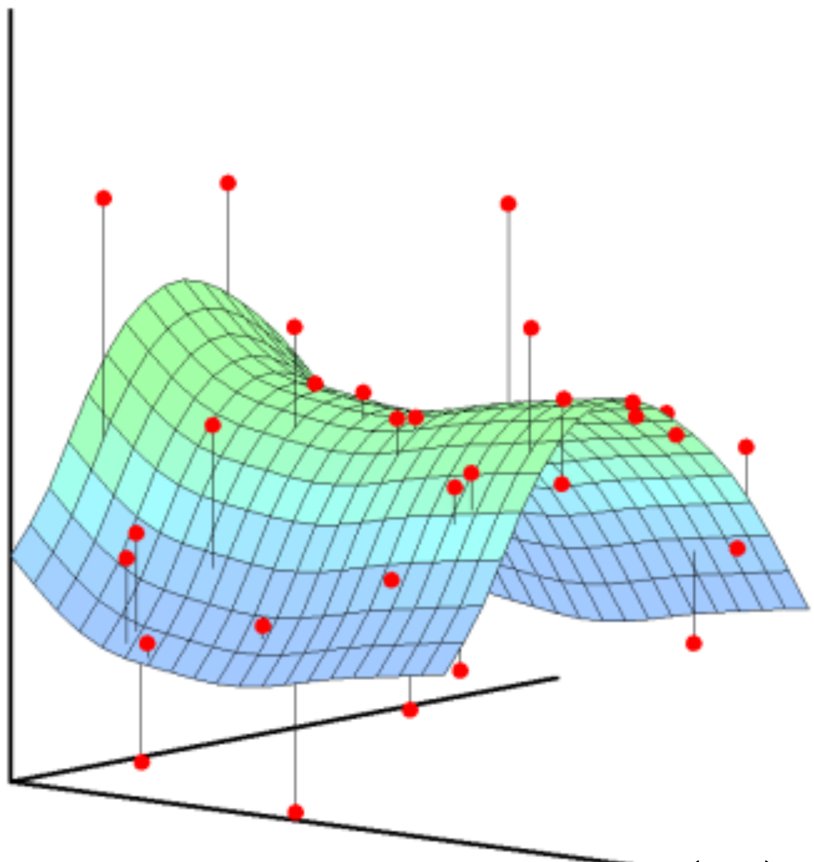
Least squares estimate:

$$\mathbf{w}^* = \mathrm{argmin}_{\mathrm{w}} L(\mathbf{w}) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Linear regression



Generalized linear regression



$$\mathbf{x} \to \boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \vdots \\ \phi_M(\mathbf{x}) \end{bmatrix}$$

Ridge regression & cross-validation

New objective:

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} + \lambda \mathbf{w}^T \mathbf{w}$$

"data fidelity"

complexity

Setting w:

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

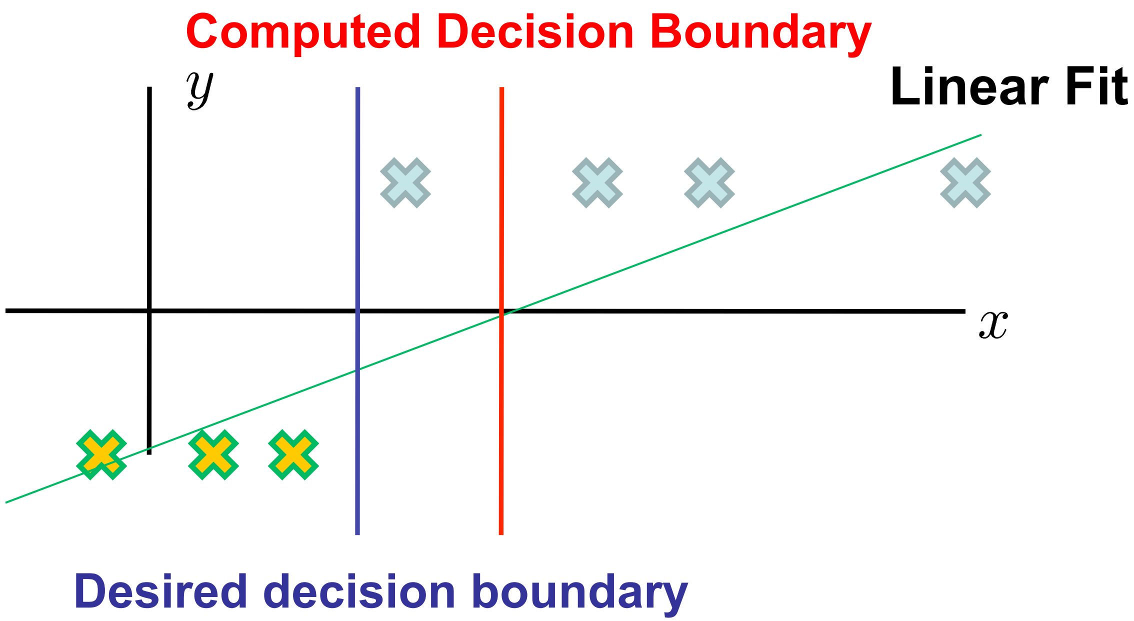
Setting λ: cross-validation

Inappropriateness of quadratic loss

We chose the quadratic cost function for convenience

Single, global minimum & closed form expression

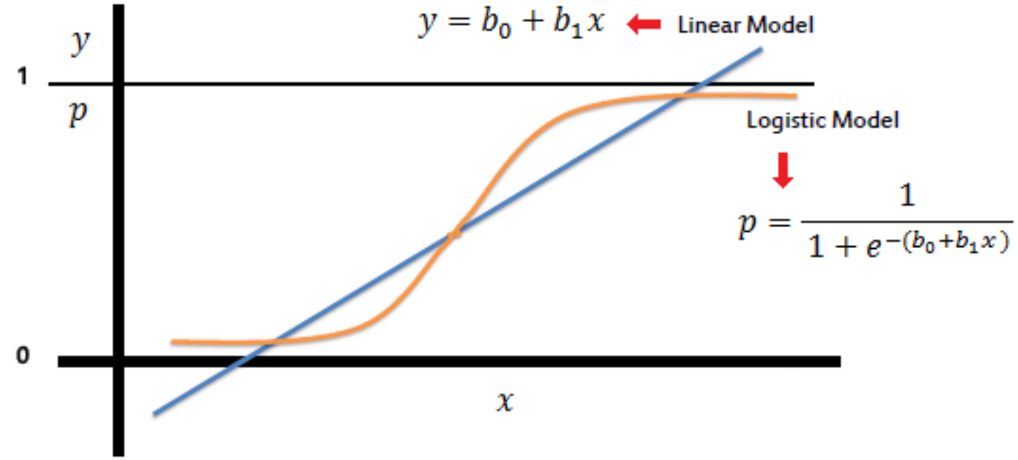
But does it indicate classification performance?

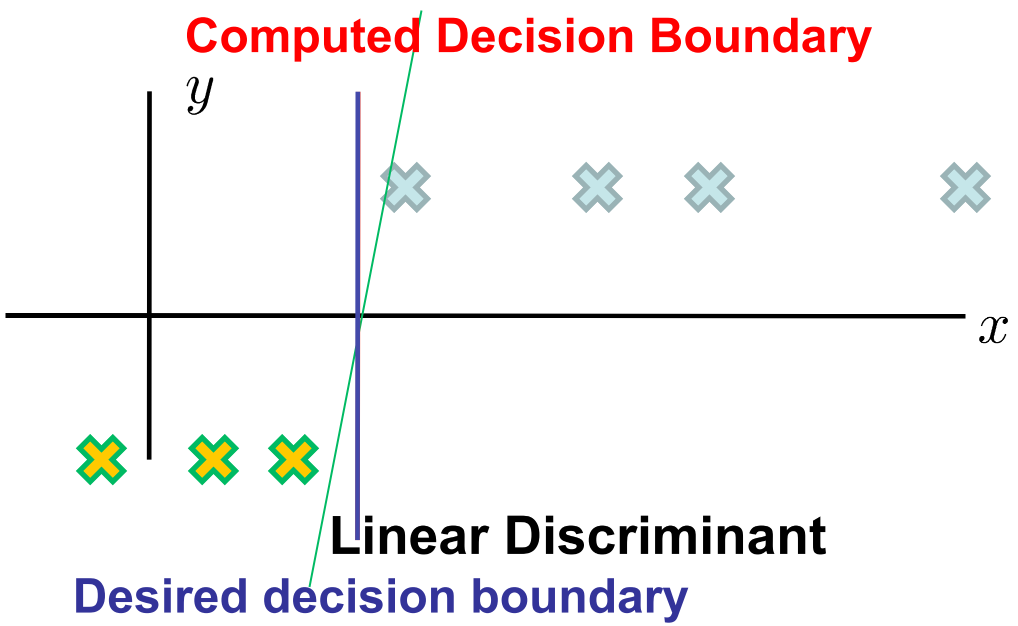


Today's basic idea

Use squashing function

The higher, the better



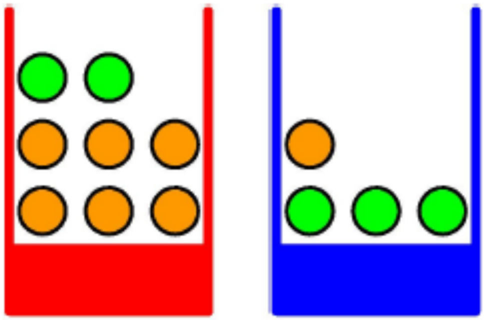


Our goal today: make this precise

Probability refresher

Probability Review -I

- Example: apples and oranges
  - We have two boxes to pick from.
  - Each box contains both types of fruit.
  - What is the probability of picking an apple?



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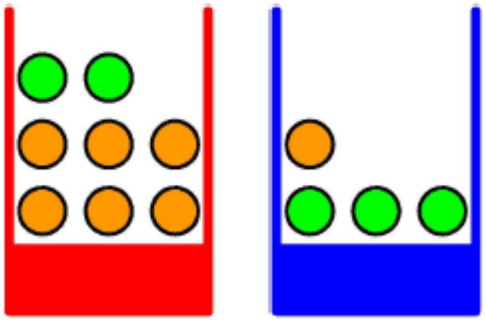


- Formalization
  - Let $B \in \{r, b\}$ be a random variable for the box we pick.
  - Let $F \in \{a, o\}$ be a random variable for the type of fruit we get.
  - Suppose we pick the red box 40% of the time. We write this as

$$p(B = r) = 0.4 \qquad p(B = b) = 0.6$$

  - The probability of picking an apple *given* a choice for the box is

$$p(F = a \mid B = r) = 0.25 \qquad p(F = a \mid B = b) = 0.75$$

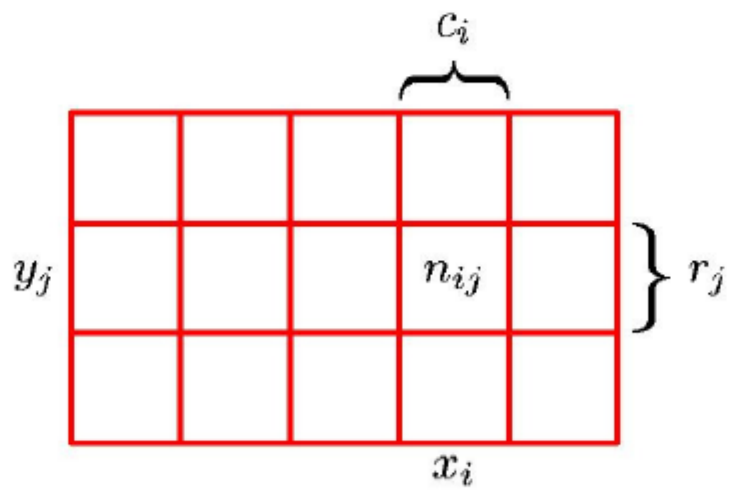
  - What is the probability of picking an apple?

$$p(F = a) = ?$$

Joint, Marginal, Conditional Probability

- More general case
  - Consider two random variables $X \in \{x_i\}$ and $Y \in \{y_j\}$
  - Consider N trials and let

$$
\begin{aligned}
n_{ij} &= \#\{X = x_i \wedge Y = y_j\} \\
c_i &= \#\{X = x_i\} \\
r_j &= \#\{Y = y_j\}
\end{aligned}
$$



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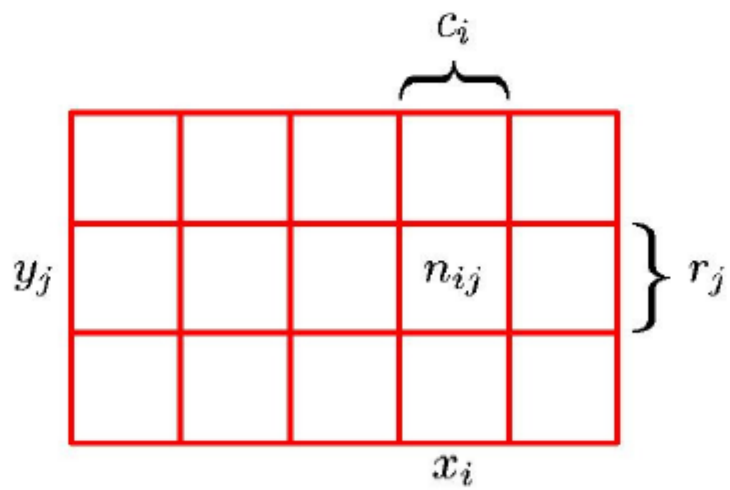


- Then we can derive
  - Joint probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

  - Marginal probability

$$p(X = x_i) = \frac{c_i}{N}.$$

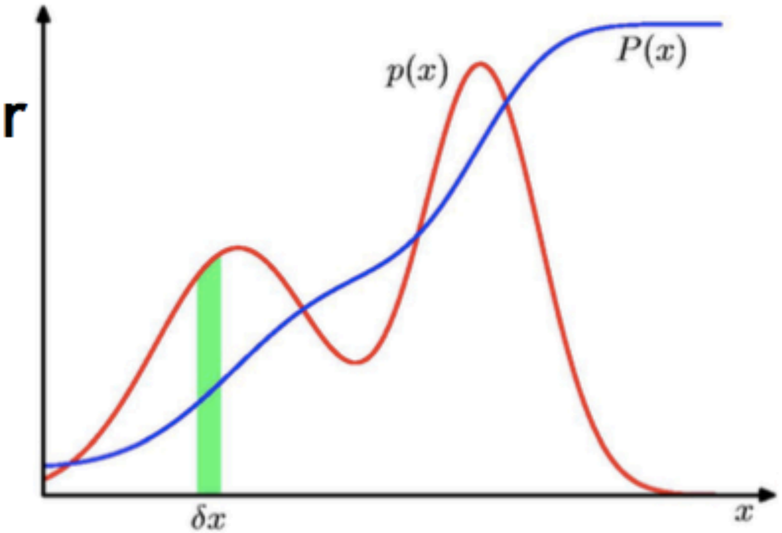
  - Conditional probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

Continuous variables

- **Probabilities over continuous variables are defined over their** **probability density function** **(pdf)** $p(x)$**.**

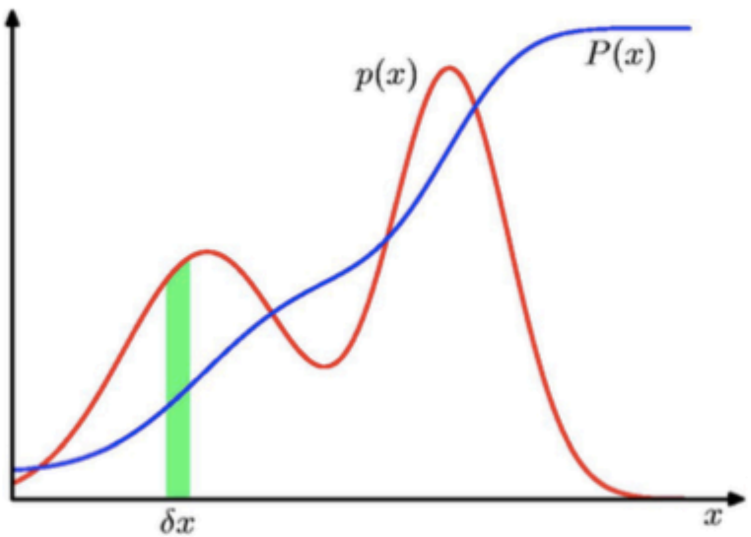
$$p(x \in (a,b)) = \int_a^b p(x)\,\mathrm{d}x$$



Continuous variables

- **Probabilities over continuous variables are defined over their probability density function (pdf) $p(x)$.**

$$p(x \in (a,b)) = \int_a^b p(x)\,\mathrm{d}x$$



- **The probability that x lies in the interval $(-\infty, z)$ is given by the cumulative distribution function**

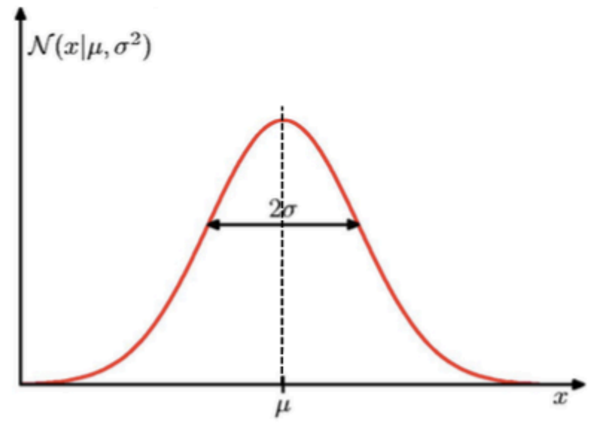
$$P(z) = \int_{-\infty}^{z} p(x)\,\mathrm{d}x$$

Gaussian (or Normal) distribution

One-dimensional case

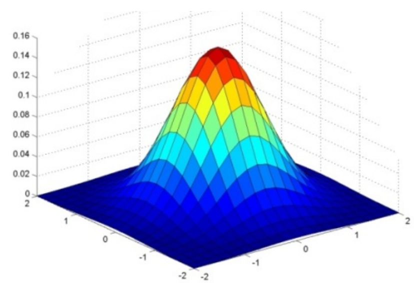
- Mean μ
- Variance σ^2

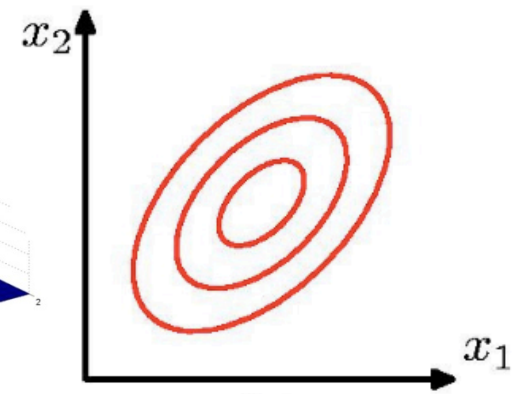
$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$



Multi-dimensional case

- Mean μ
- Covariance Σ



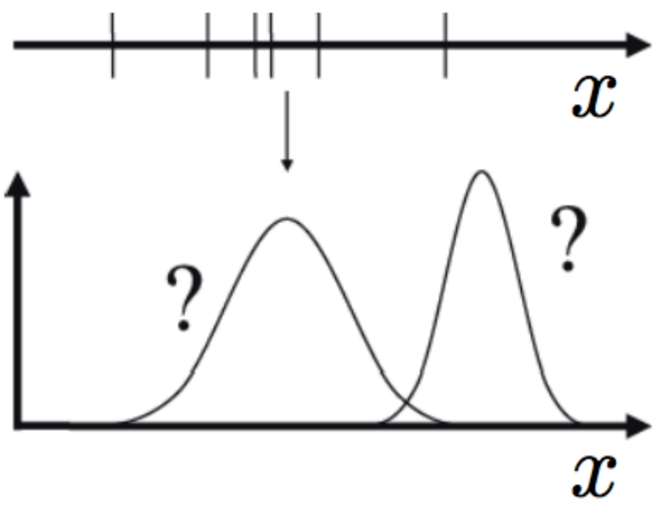


$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Parameter estimation

Given

- Data $X = \{x_1, x_2, \ldots, x_N\}$
- Parametric form of the distribution with parameters θ
- E.g. for Gaussian distrib.: $\theta = (\mu, \sigma)$



Learning

- Estimation of the parameters θ

Parameter estimation

Given

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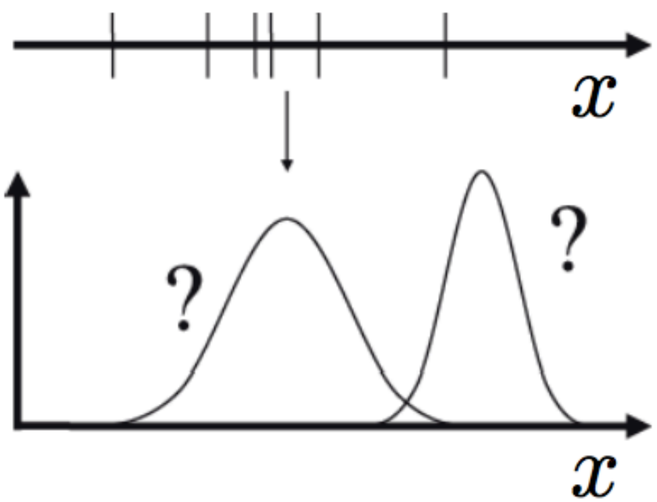

Learning

- Estimation of the parameters θ

Likelihood of θ

- Probability that the data X have indeed been generated from a probability density with parameters θ

$$L(\theta) = p(X|\theta)$$

Computation of the likelihood

- Single data point: $p(x_n|\theta)$

Computation of the likelihood

- Single data point: $p(x_n|\theta)$

- Assumption: all data points are independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

Computation of the likelihood

- Single data point: $p(x_n|\theta)$

- Assumption: all data points are independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

- Negative (of) log-likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

Computation of the likelihood

- Single data point: $p(x_n|\theta)$
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$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

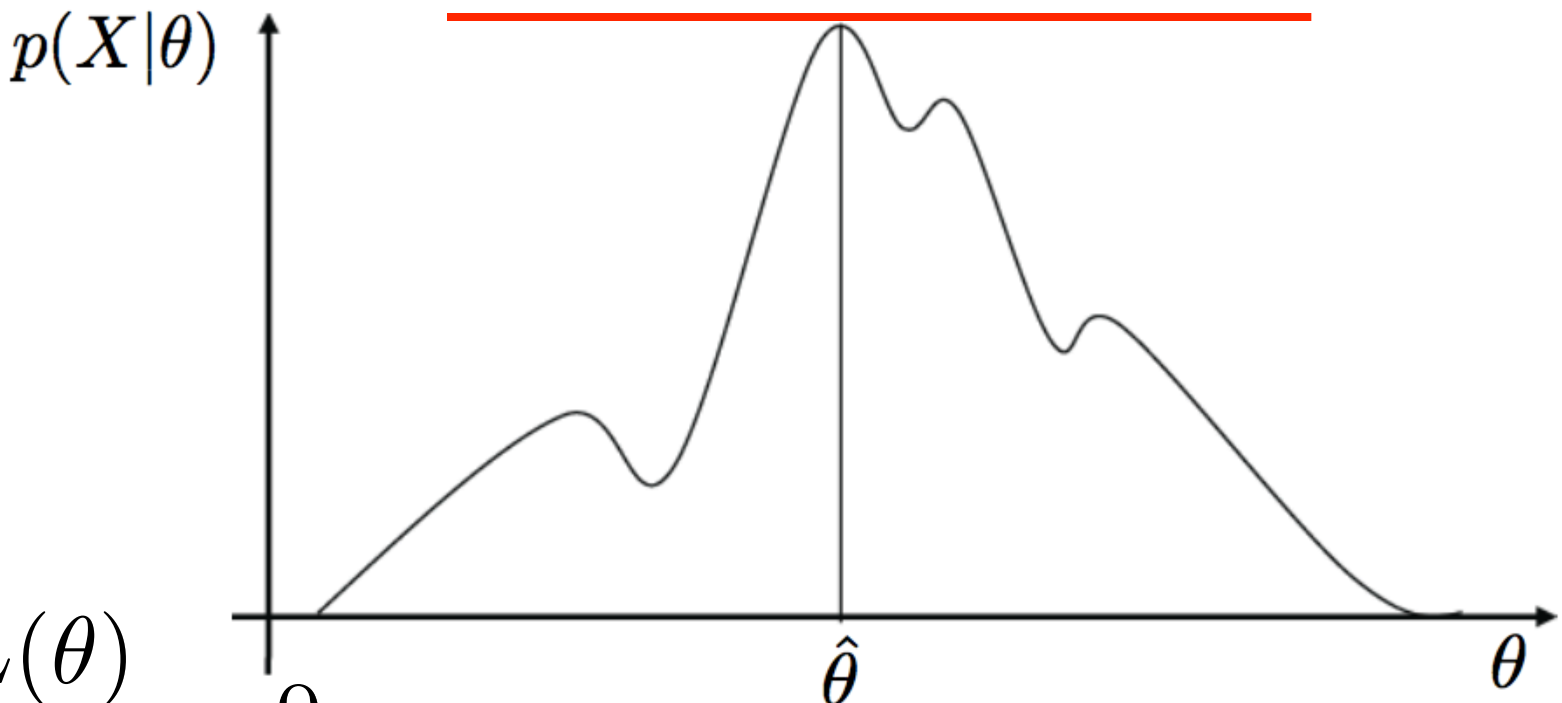
- Negative (of) log-likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

- Estimation of the parameters θ (Learning)
  - Maximize the likelihood
  - Minimize the negative log-likelihood

Likelihood: $$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

We want to obtain $\hat{\theta}$ such that $L(\hat{\theta})$ is maximized.

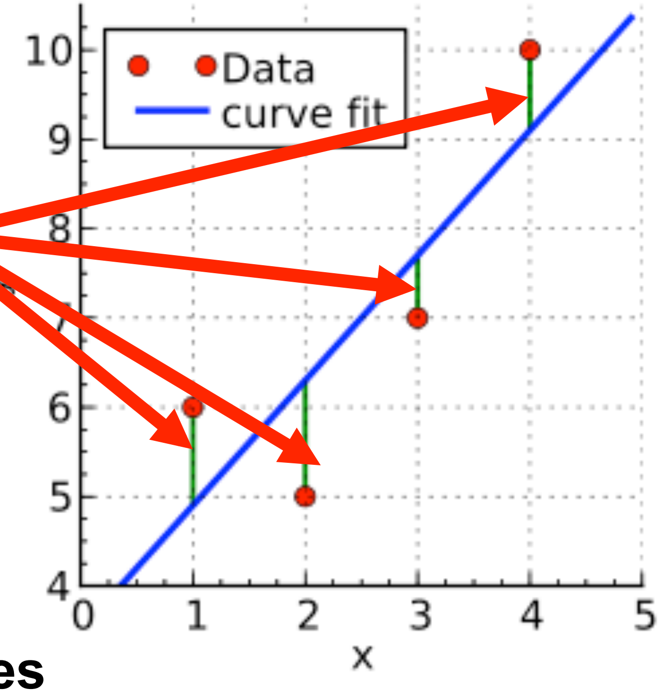


$$\frac{\partial L(\theta)}{\partial \theta} = 0$$

Probabilistic formulation of linear regression-I

$$\epsilon^i = y^i - \mathbf{w}^T \mathbf{x}^i$$

residuals



Residual: zero-mean Gaussian random variable

$$p(E^i = \epsilon^i) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(\epsilon^i)^2}{2\sigma^2}\right)$$

The R.V. **its value**

random variables

$$Y^i = \mathbf{w}^T \mathbf{x}^i + E^i$$

deterministic

Conditional model on observations:

$$p(Y^i = y^i | \mathbf{x}^i; \mathbf{w}^T) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y^i - \mathbf{w}^T \mathbf{x}^i)^2}{2\sigma^2}\right)$$

Probabilistic interpretation of linear regression

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \mathbb{R}$

$$p(y^1, \ldots, y^n | \mathbf{x}^1, \ldots, \mathbf{x}^N) =$$

Independence assumption

$$= \prod_{i=1}^{N} p(y^i | \mathbf{x}^i)$$

$$= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^i - \mathbf{w}^T \mathbf{x}^i)^2}{2\sigma^2}\right)$$

$$= \frac{1}{(\sqrt{2\pi}\sigma)^N} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2\right)$$

=> Least squares: Maximum Conditional Likelihood estimation of w

Great, but only for real-valued outputs!

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \mathbb{R}$

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From regression to classification

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \{0, 1\}$

$$p(y^1, \ldots, y^n | \mathbf{x}^1, \ldots, \mathbf{x}^N) =$$

Independence assumption

$$= \prod_{i=1}^{N} p(y^i | \mathbf{x}^i)$$

?

Bernoulli distribution

Discrete random variable $Y \in \{0, 1\}$

1x2 table, 1 parameter:

$$P(Y = 1) = p$$
$$P(Y = 0) = 1 - P(Y = 1) = 1 - p$$

Compact form:

$$P(Y = c) = \begin{cases} p & c = 1 \\ 1 - p & c = 0 \end{cases}$$
$$= p^c (1 - p)^{1-c}$$

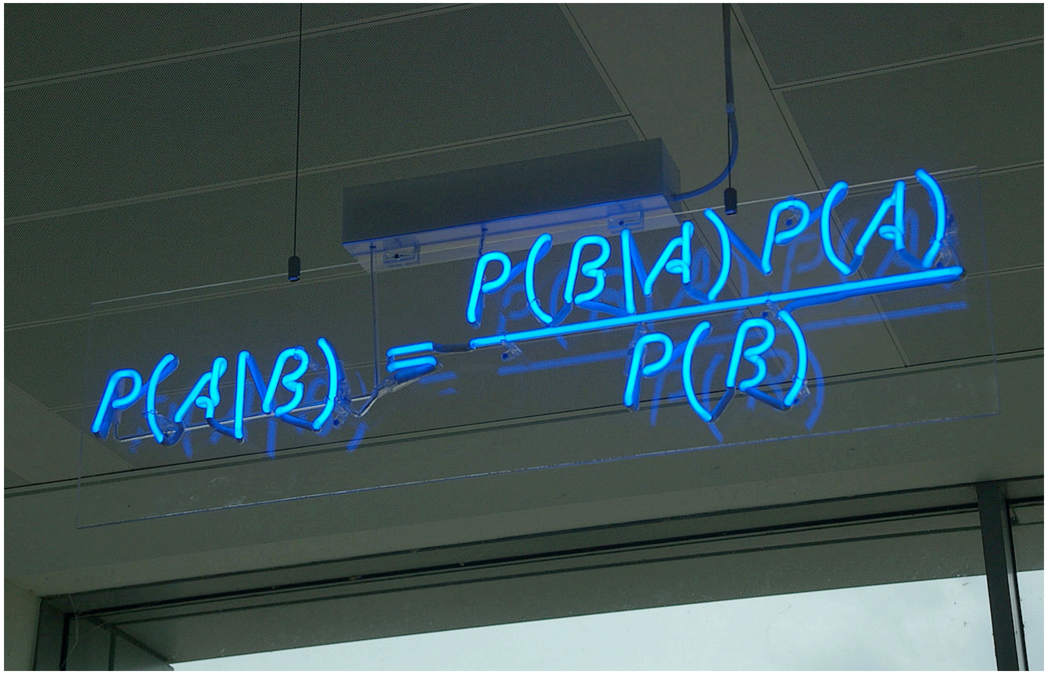
Parametric model for posterior

$$P(Y=1|X=\mathbf{x};\mathbf{w}) = f(\mathbf{x},\mathbf{w})$$
$$P(Y=0|X=\mathbf{x};\mathbf{w}) = 1 - f(\mathbf{x},\mathbf{w})$$

$$P(Y=y|X=\mathbf{x};\mathbf{w}) = f(\mathbf{x},\mathbf{w})^y(1-f(\mathbf{x},\mathbf{w}))^{1-y}$$

What would be a reasonable expression for f?

Bayes' rule



Sum and product rule

Sum Rule $$p(X) = \sum_Y p(X, Y)$$

Product Rule $$p(X, Y) = p(Y|X)p(X)$$

Bayes' theorem

$$P(A = a, B = b) = P(A = a, B = b)$$

Product rule:

$$P(A = a|B = b)P(B = b) = P(B = b|A = a)P(A = a)$$

$$P(A = a|B = b) = \frac{P(B{=}b|A{=}a)P(A{=}a)}{P(B{=}b)}$$

Sum rule:

$$P(A = a|B = b) = \frac{P(B = b|A = a)P(A = a)}{\sum_{a'} P(B = b, A = a')}$$

Product rule:

$$P(A = a|B = b) = \frac{P(B = b|A = a)P(A = a)}{\sum_{a'} P(B = b|A = a')P(A = a')}$$

Bayes' theorem

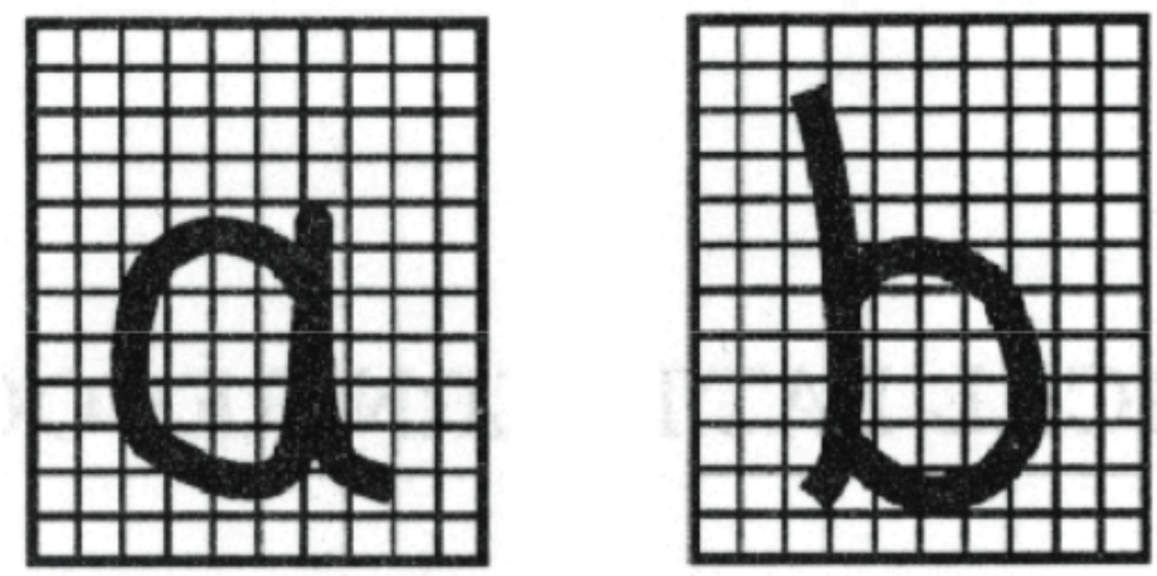
Sum Rule	$p(X) = \sum_{Y} p(X, Y)$
Product Rule	$p(X, Y) = p(Y\|X)p(X)$

- From those, we can derive

Bayes' Theorem	$p(Y\|X) = \frac{p(X\|Y)p(Y)}{p(X)}$
where	$p(X) = \sum_{Y} p(X\|Y)p(Y)$

Binary classification problem

- Example: handwritten character recognition



- Goal:
  - Classify a new letter such that the probability of misclassification is minimized.

Binary classification problem

- **Concept 1: Priors (a priori probabilities)** $p(C_k)$
  - **What we can tell about the probability *before seeing the data*.**

Binary classification problem

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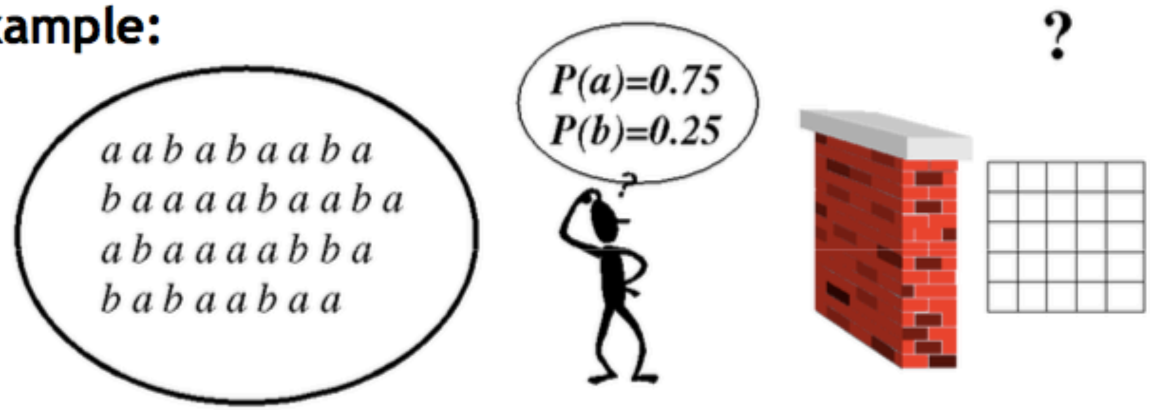
  - What we can tell about the probability *before seeing the data.*
  - Example:



$$C_1 = a \qquad p(C_1) = 0.75$$

$$C_2 = b \qquad p(C_2) = 0.25$$

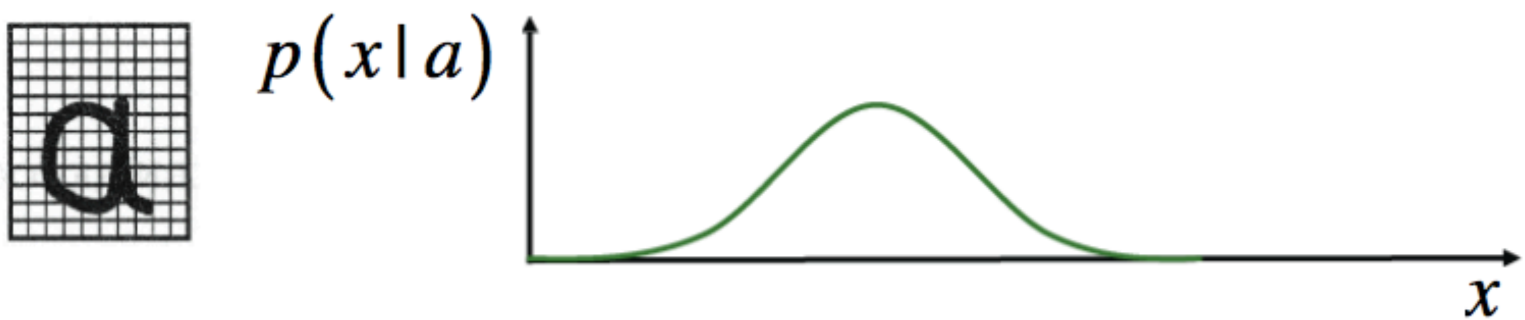
- **In general:** $\sum_k p(C_k) = 1$

Binary classification problem

Concept 2: Conditional probabilities

$$p(x \mid C_k)$$

- Let x be a feature vector.
- x measures/describes certain properties of the input.
  - E.g. number of black pixels, aspect ratio, …
- $p(x|C_k)$ describes its likelihood for class C_k.



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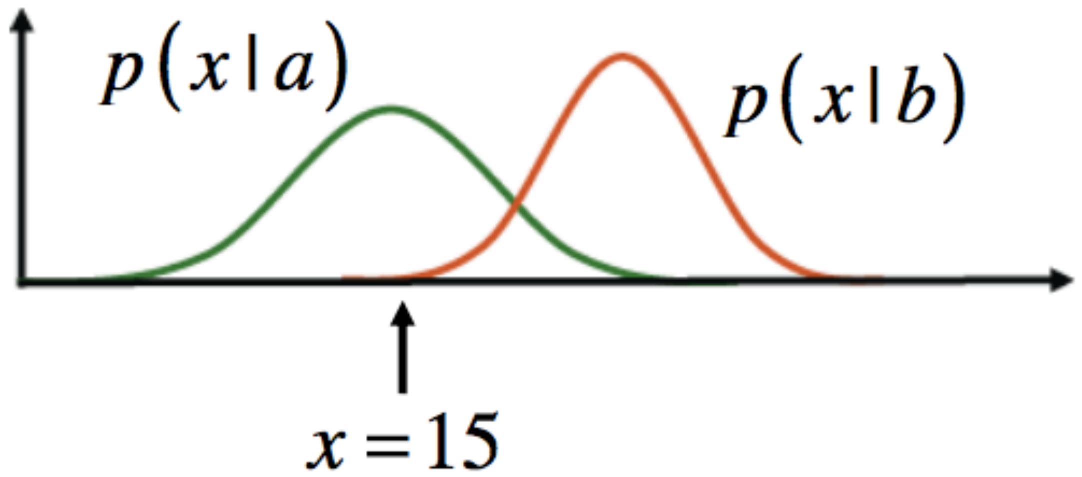

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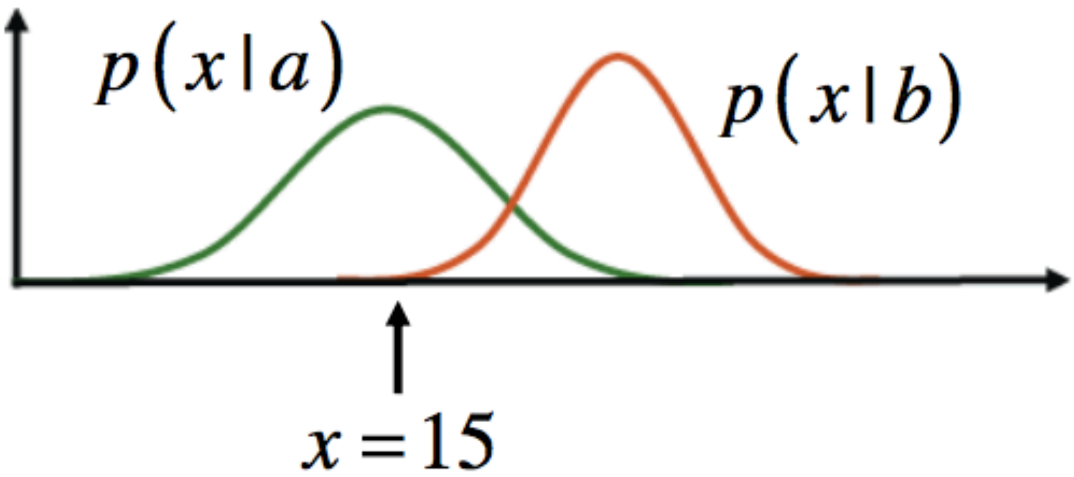
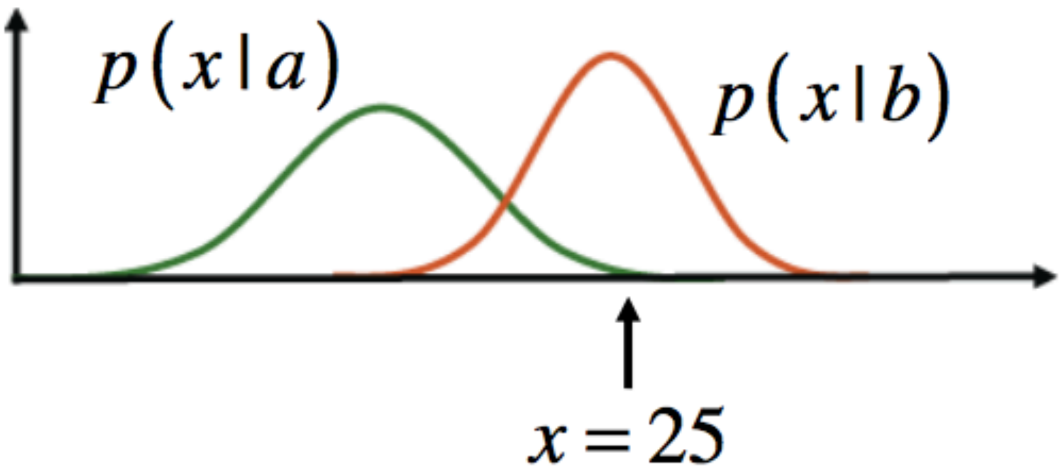


Question:

- Which class?
- The decision should be ‘a’ here.

Example:



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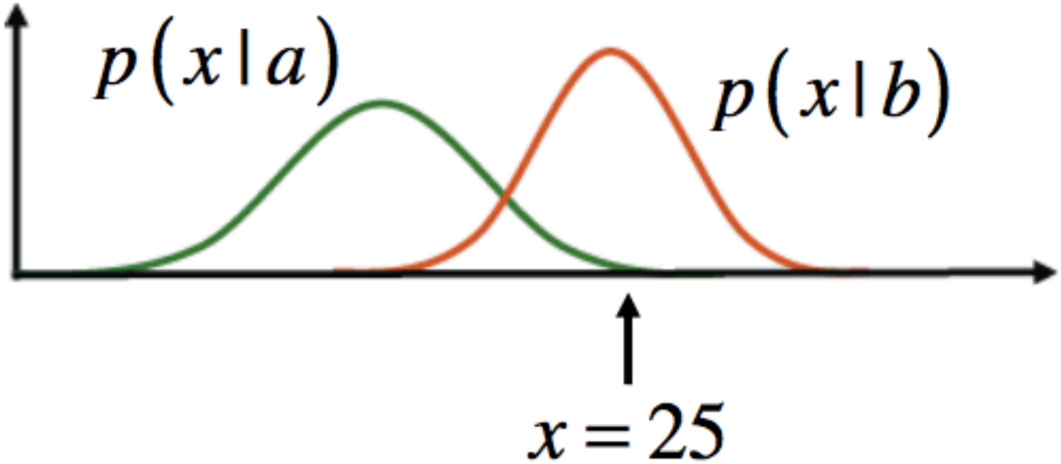
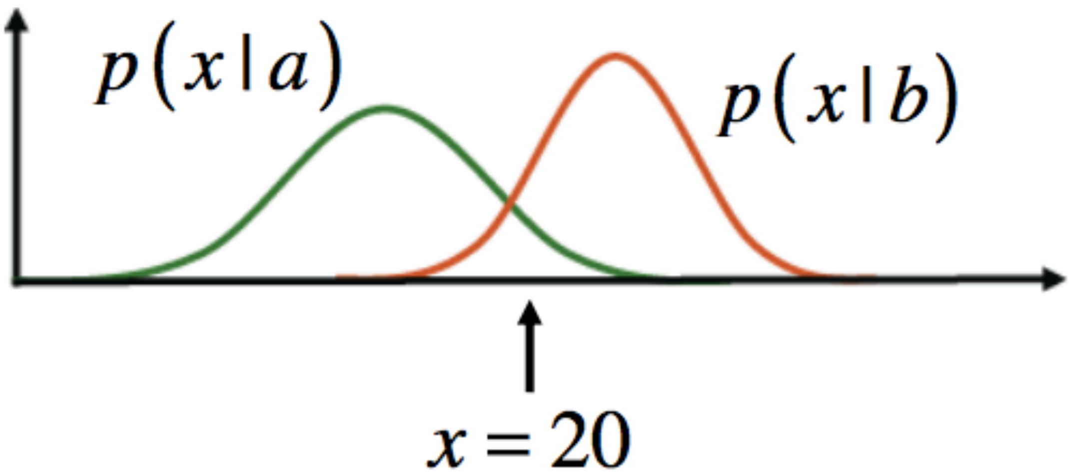


Question:

- Which class?
- Since $p(x|a)$ is much smaller than $p(x|b)$, the decision should be ‘b’ here.

Example:



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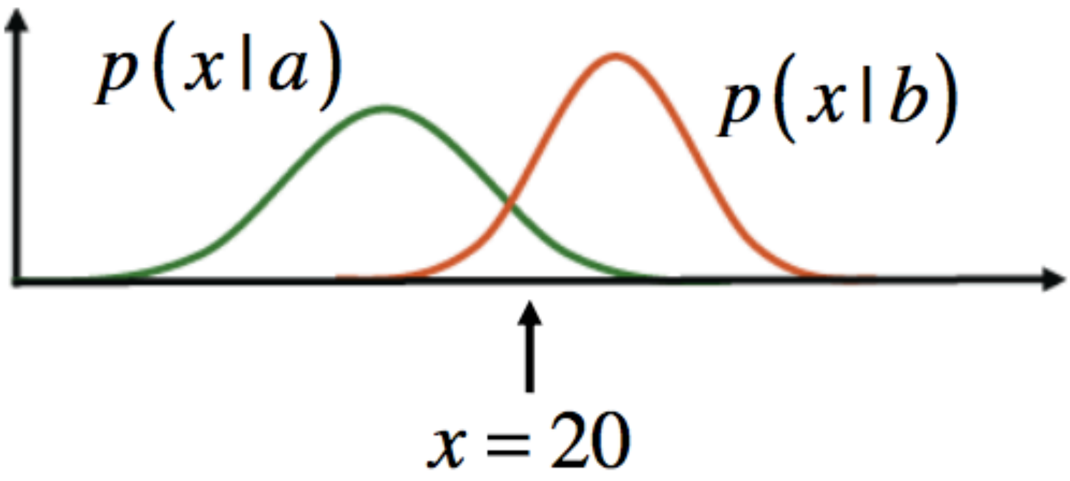


Question:

- Which class?
- Remember that $p(a) = 0.75$ and $p(b) = 0.25$...
- I.e., the decision should be again 'a'.

$\Rightarrow$ How can we formalize this?

Concept 3: Posterior probabilities

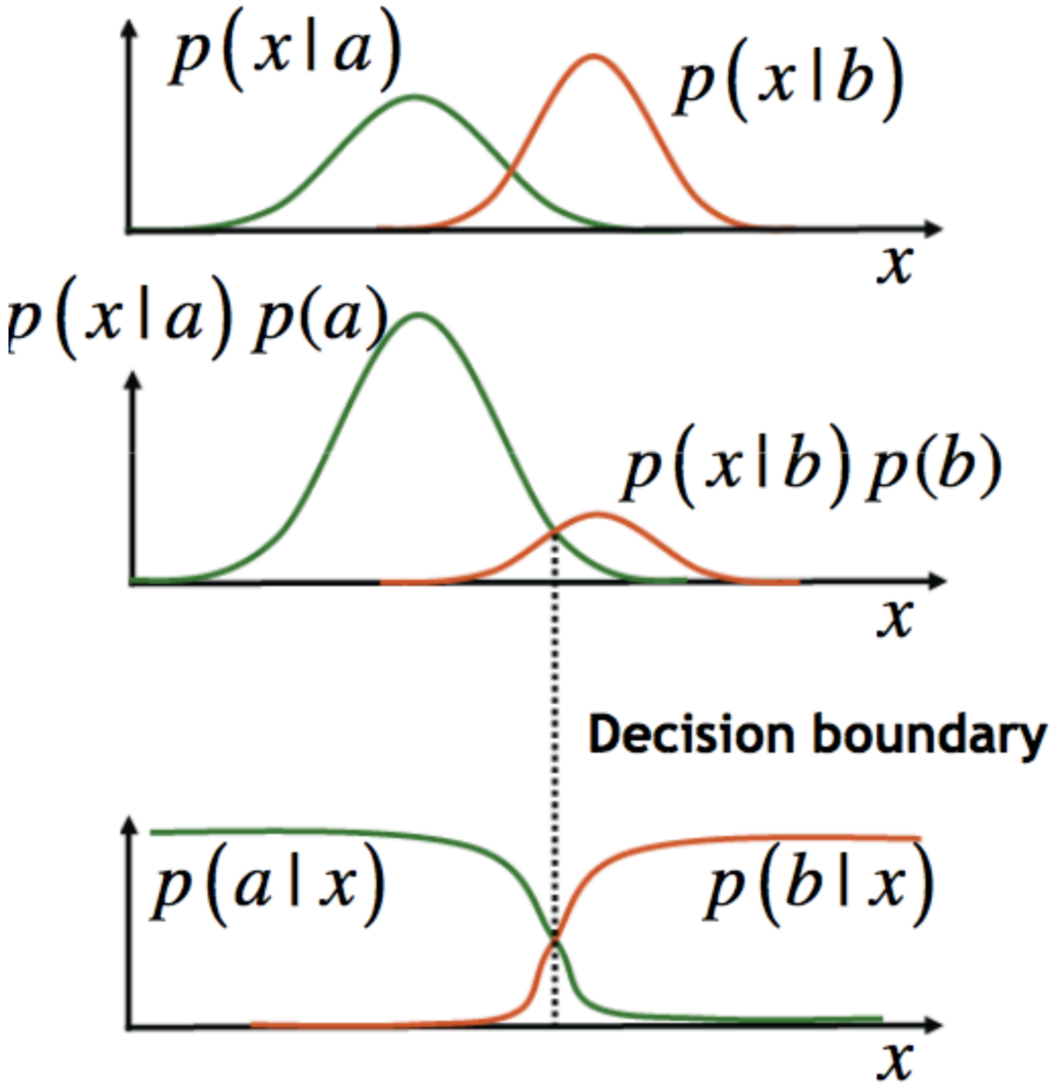
$$p(C_k \mid x)$$

- We are typically interested in the *a posteriori* probability, i.e. the probability of class C_k given the measurement vector x.

Bayes' Theorem:

$$p(C_k \mid x) = \frac{p(x \mid C_k)\, p(C_k)}{p(x)} = \frac{p(x \mid C_k)\, p(C_k)}{\sum_i p(x \mid C_i)\, p(C_i)}$$

Bayes' rule for binary classification problem



Probability of observation, conditioned on class

Probability of class, conditioned on observation ('posterior')

Binary Classification for Gaussian distributions

Assumption: within each class, features follow a Gaussian distribution

$$p(\mathbf{X}=\mathbf{x}|y=c)=\frac{1}{\sqrt{2\pi}^N|\Sigma_c|^{1/2}}\exp\left(-\frac{1}{2}(\mathbf{x}-\mu_c)^T\Sigma_c^{-1}(\mathbf{x}-\mu_c)^T\right)$$

Shortcut notation: $p(\mathbf{x}|c)$ instead of $p(\mathbf{X}=\mathbf{x}|C=c)$

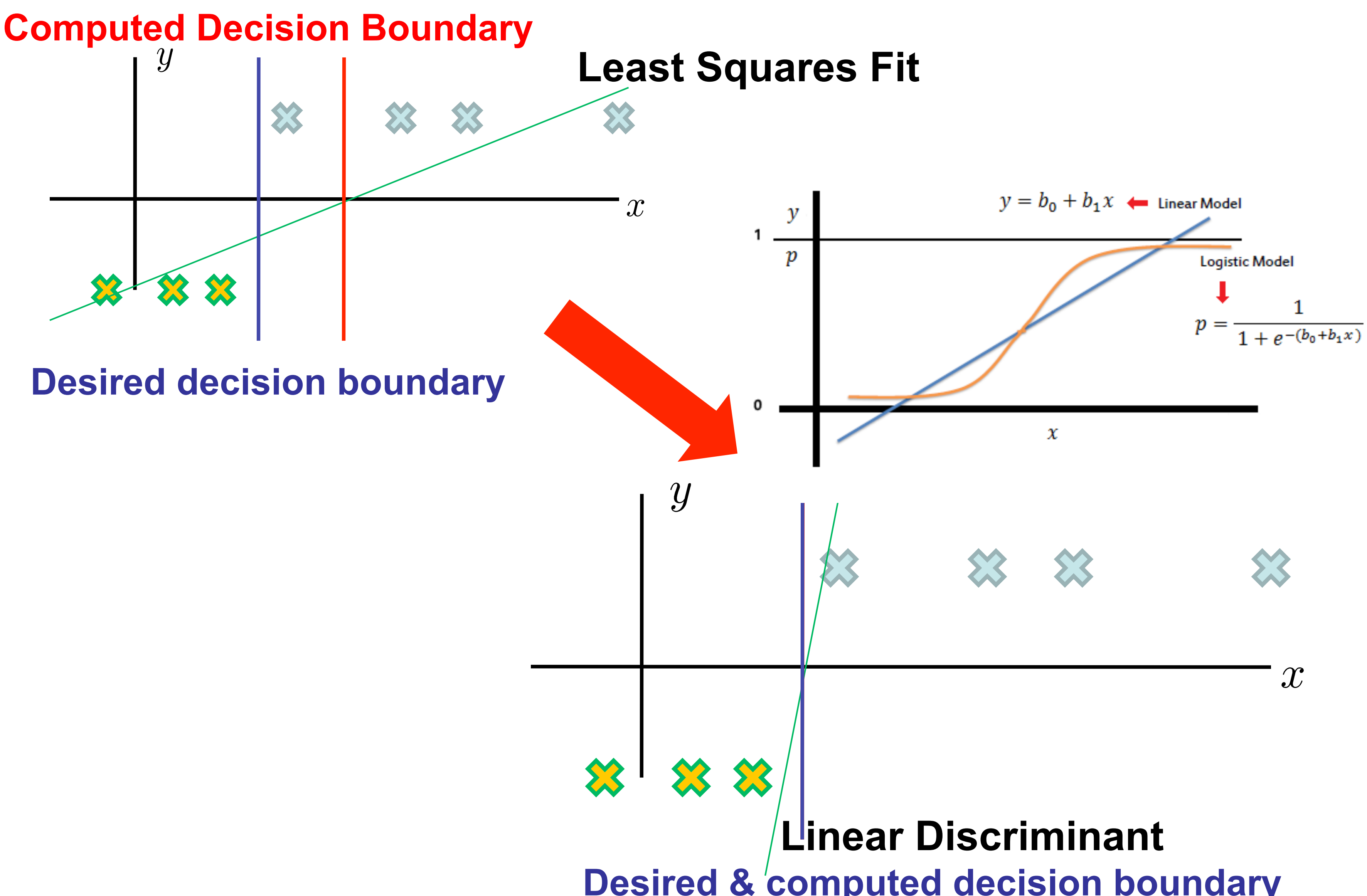
Posterior: $$p(1|\mathbf{x})=\frac{p(\mathbf{x}|1)p(1)}{\sum_{c\in\{0,1\}}p(\mathbf{x}|c)p(c)}$$

Special case: $\Sigma=\Sigma_0=\Sigma_1$

$$p(1|\mathbf{x})=\frac{1}{1+\exp\left(-(\mathbf{w}^T\mathbf{x}+b)\right)}$$

$$\mathbf{w}=\Sigma^{-1}(\mu_1-\mu_0)\qquad b=\frac{1}{2}(\mu_0^T\Sigma^{-1}\mu_0-\mu_1^T\Sigma^{-1}\mu_1)$$

Back to classification



From regression to classification

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \{0, 1\}$

$$p(y^1, \ldots, y^n | \mathbf{x}^1, \ldots, \mathbf{x}^N) =$$

Independence assumption

$$= \prod_{i=1}^{N} p(y^i | \mathbf{x}^i)$$

?

Form of posterior distribution

Bernoulli-type conditional distribution

$$\left.\begin{array}{rl} P(Y=1|X=\mathbf{x};\mathbf{w}) = & f(\mathbf{x},\mathbf{w}) \\ P(Y=0|X=\mathbf{x};\mathbf{w}) = & 1-f(\mathbf{x},\mathbf{w}) \end{array}\right\} \rightarrow$$

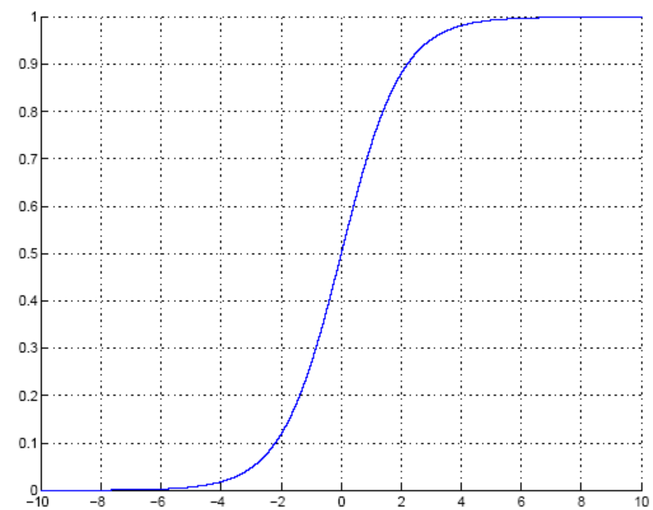
$$P(Y=y|X=\mathbf{x};\mathbf{w}) = f(\mathbf{x},\mathbf{w})^y(1-f(\mathbf{x},\mathbf{w}))^{1-y}$$

Particular choice of form of f:

$$P(Y=1|X=\mathbf{x};\mathbf{w}) = g(\mathbf{w}^T\mathbf{x})$$

Sigmoidal: $g(\alpha) = \dfrac{1}{1+\exp(-a)}$

"squashing function": $\begin{array}{l} -\infty \rightarrow 0 \\ +\infty \rightarrow 1 \end{array}$



From regression to classification, continued

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}, \mathbf{x} \in \mathbb{R}^D, y \in \{0,1\}$

$$p(y^1, \ldots, y^n | \mathbf{x}^1, \ldots, \mathbf{x}^N) =$$

Independence assumption

$$= \prod_{i=1}^{N} P(y^i|\mathbf{x}^i)$$

$$= \prod_{i=1}^{N} g(\mathbf{w}^T\mathbf{x}^i)^{y^i}(1 - g(\mathbf{w}^T\mathbf{x}^i))^{1-y^i}$$

$$\log P(\mathbf{y}|\mathbf{X};\mathbf{w}) = \sum_{i=1}^{N} \log\left(g(\mathbf{w}^T\mathbf{x}^i)^{y^i}\right) + \log\left(\left(1 - g(\mathbf{w}^T\mathbf{x}^i)\right)^{(1-y^i)}\right)$$

$$= \sum_{i=1}^{N} y^i \log g(\mathbf{w}^T\mathbf{x}^i) + (1-y^i)\log(1 - g(\mathbf{w}^T\mathbf{x}^i))$$

Q1: How does this behave? Q2: How to optimize it with respect to w?

Loss function for linear regression

Training: given $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$, estimate optimal $\mathbf{w}$

Loss function: quantify appropriateness of $\mathbf{w}$

$$L(S, \mathbf{w}) = \sum_{i=1}^{N} l(y^i, f_{\mathbf{w}}(\mathbf{x}^i))$$

$$= \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 = \sum_{i=1}^{N} (\epsilon^i)^2$$

Loss function for classification

Training: given $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$, estimate optimal $\mathbf{w}$

Loss function: quantify appropriateness of $\mathbf{w}$

$$L(S, \mathbf{w}) = -\log P(\mathbf{y}|\mathbf{X}; \mathbf{w})$$

$$= -\sum_{i=1}^{N} \log P(y^i|\mathbf{x}^i; \mathbf{w})$$

$$= -\sum_{i=1}^{N} y^i \log g(\mathbf{w}^T\mathbf{x}^i) + (1 - y^i) \log(1 - g(\mathbf{w}^T\mathbf{x}^i))$$

$$= \sum_{i=1}^{N} l(y^i, f_{\mathbf{w}}(\mathbf{x}^i))$$

Linear discriminant: $f_{\mathbf{w}}(\mathbf{x}^i) = \mathbf{w}^T\mathbf{x}^i$

Rewriting the quadratic loss

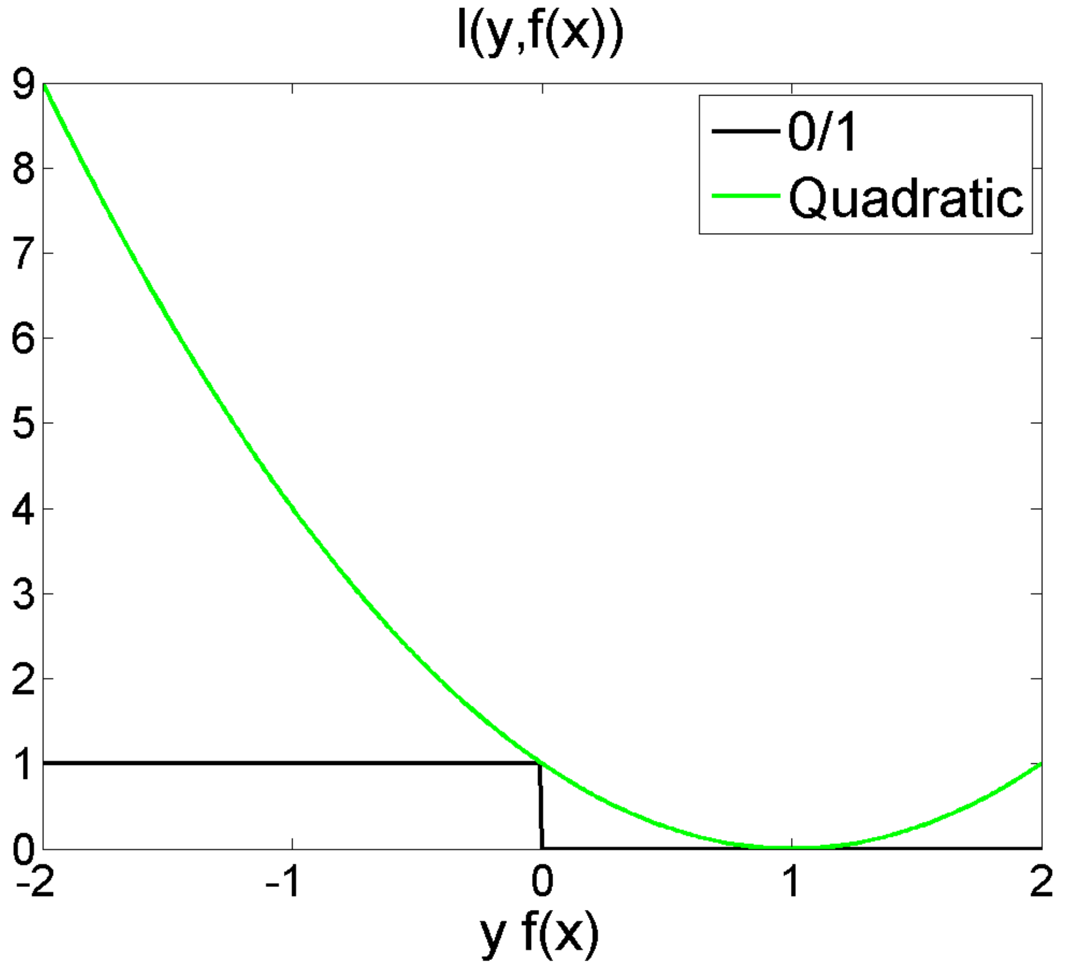
Consider transformation: $y_{\pm} = 2y_b - 1$

$y_b \in \{0, 1\} \qquad y_{\pm} \in \{-1, 1\}$

$$
\begin{aligned}
l(y, f_{\mathbf{w}}(\mathbf{x})) &= (y - f_{\mathbf{w}}(\mathbf{x}))^2 \\
&\overset{y^2=1}{=} y^2(y - f_{\mathbf{w}}(\mathbf{x}))^2 \\
&= (y^2 - y f_{\mathbf{w}}(\mathbf{x}))^2 \\
&\overset{y^2=1}{=} (1 - y f_{\mathbf{w}}(\mathbf{x}))^2
\end{aligned}
$$

Inappropriateness of quadratic loss for classification

Last slide: $l(y, f(x)) = (1 - yf(x))^2$



Quadratic loss is not robust to outliers and penalizes outputs that are `too good'

Rewriting the cross-entropy loss

As before: $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ $\quad y_{\pm} = 2y_b - 1 \quad y_b \in \{0, 1\}$

$y_{\pm} \in \{-1, 1\}$

$$P(Y = 1 | X = \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-h_{\mathbf{w}}(\mathbf{x}))}$$

$$P(Y = -1 | X = \mathbf{x}; \mathbf{w}) = 1 - P(Y = 1 | X = \mathbf{x}; \mathbf{w})$$

$$= 1 - \frac{1}{1 + \exp(-h_{\mathbf{w}}(\mathbf{x}))}$$

$$= \frac{\exp(-h_{\mathbf{w}}(\mathbf{x}))}{1 + \exp(-h_{\mathbf{w}}(\mathbf{x}))}$$

$$= \frac{1}{1 + \exp(h_{\mathbf{w}}(\mathbf{x}))}$$

Rewriting the cross-entropy loss

As before: $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$ $\quad y_{\pm} = 2y_b - 1 \quad y_b \in \{0, 1\}$

Last slide: $\quad y_{\pm} \in \{-1, 1\}$

$$P(Y = 1 | X = \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-h_{\mathbf{w}}(\mathbf{x}))}$$

$$P(Y = -1 | X = \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(h_{\mathbf{w}}(\mathbf{x}))}$$

Compact form:

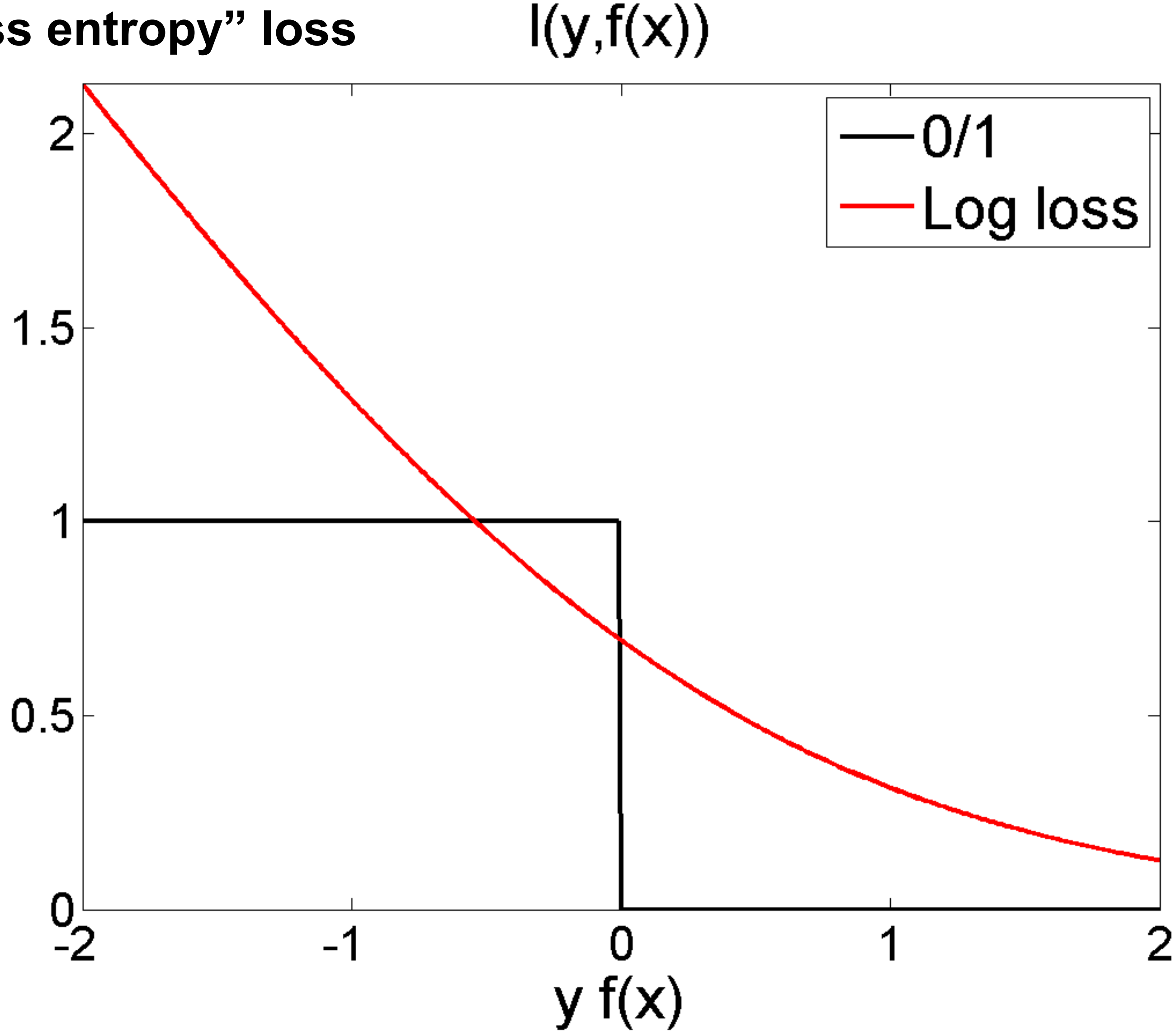
$$P(Y = y | X = \mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-y h_{\mathbf{w}}(\mathbf{x}))}$$

$$L(S, \mathbf{w}) = \sum_{i=1}^{N} -\log P(Y = y^i | X = \mathbf{x}^i; \mathbf{w})$$

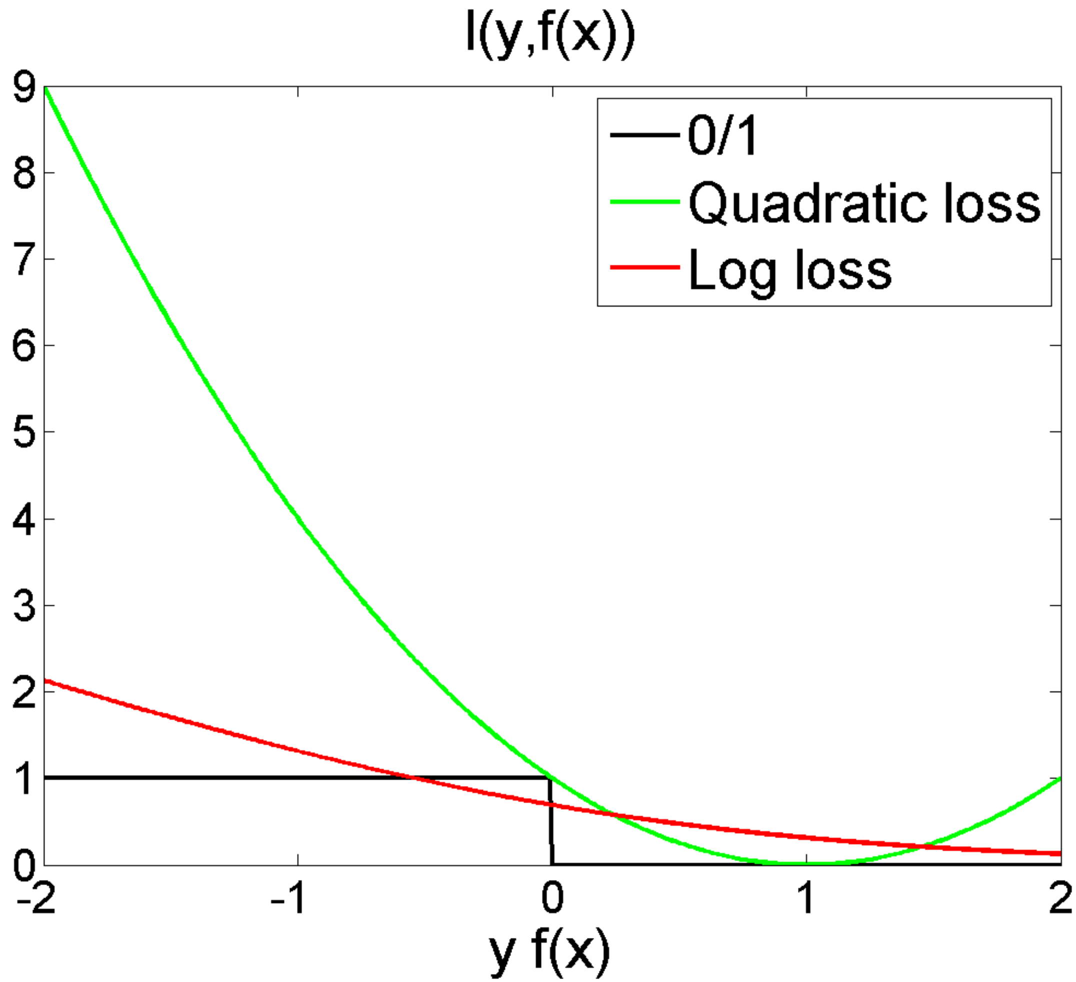
$$= \sum_{i=1}^{N} \log(1 + \exp(-y^i h_{\mathbf{w}}(\mathbf{x}^i)))$$

Log loss: $l(y, f(x)) = \log(1 + \exp(-yf(x)))$

a.k.a. "cross entropy" loss



Log loss vs. quadratic loss



Quadratic loss

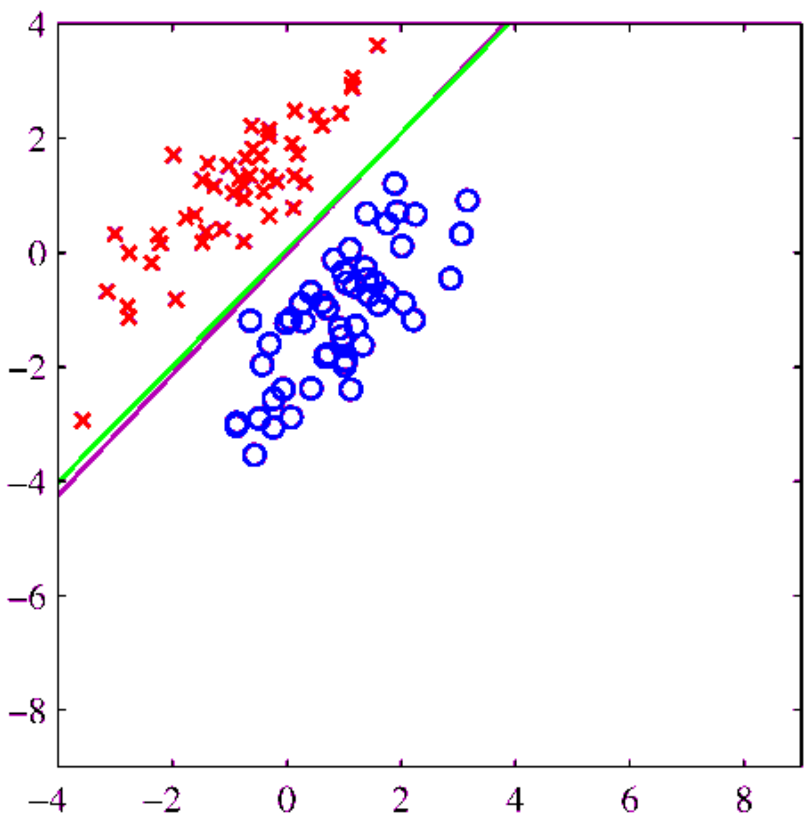
$$l(y, f(x)) = (1 - yf(x))^2$$

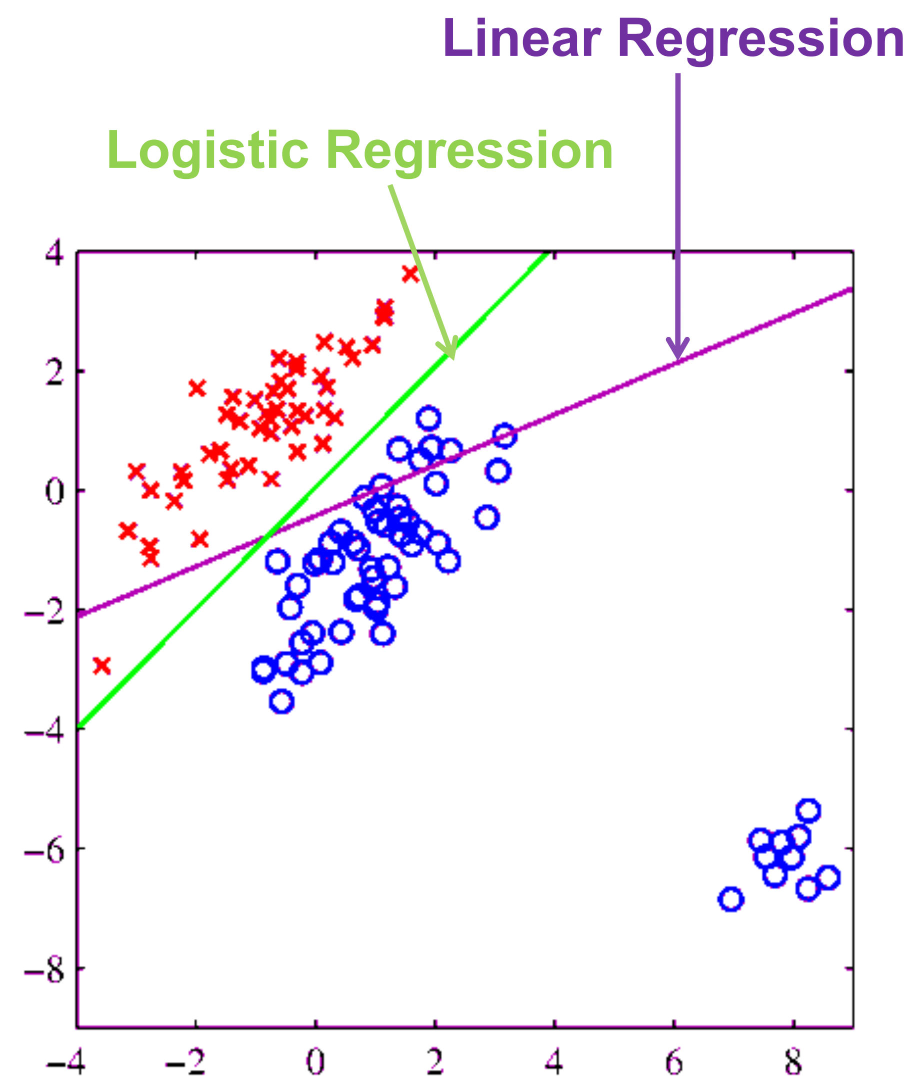
Log loss

$$l(y, f(x)) = \log(1 + \exp(-yf(x)))$$

Logistic vs Linear Regression

Logistic regression is more robust





From two to many

- So far: binary classification
- How about multi-class classification?

Multiple classes & linear regression

C classes: one-of-c coding (or one-hot encoding)

4 classes, i-th sample is in 3rd class: $\mathbf{y}^i = (0,0,1,0)$

Matrix notation:

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}^1 \\ \hline \vdots \\ \hline \mathbf{y}^N \end{bmatrix} = \left[\; \mathbf{y}_1 \; \middle| \; \ldots \; \middle| \; \mathbf{y}_C \; \right] \qquad \text{where} \quad \mathbf{y}_c = \begin{bmatrix} y_c^1 \\ \vdots \\ y_c^N \end{bmatrix}$$

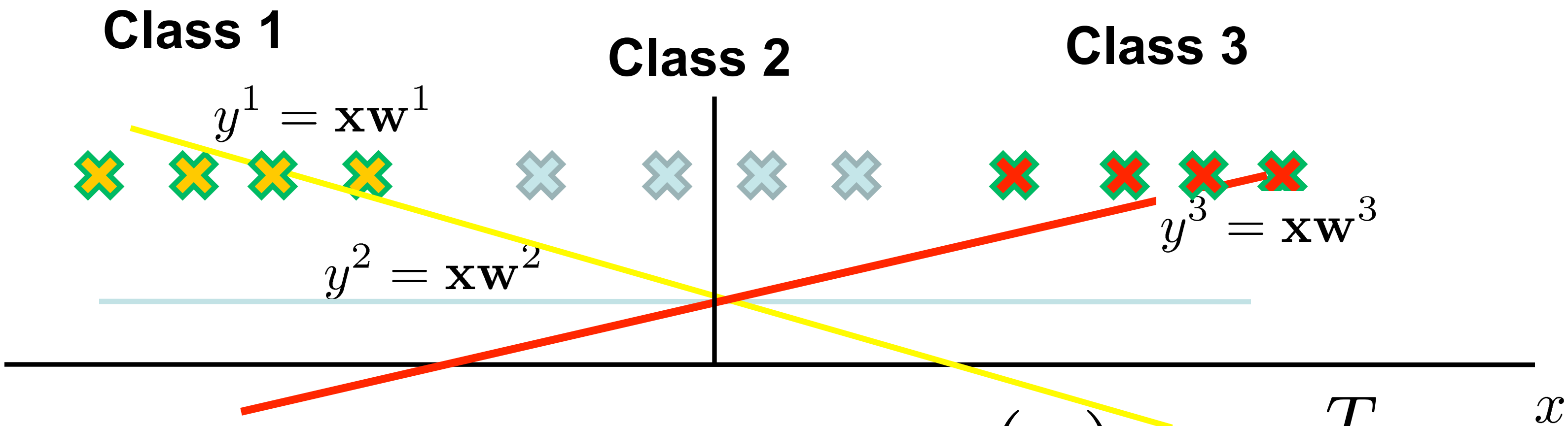
$$\mathbf{W} = \left[\; \mathbf{w}_1 \; \middle| \; \ldots \; \middle| \; \mathbf{w}_C \; \right]$$

Loss function: $$L(\mathbf{W}) = \sum_{c=1}^{C} (\mathbf{y}_c - \mathbf{X}\mathbf{w}_c)^T (\mathbf{y}_c - \mathbf{X}\mathbf{w}_c)$$

Least squares fit (decouples per class):

$$\mathbf{w}_c^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \mathbf{X}^T \mathbf{y}_c$$

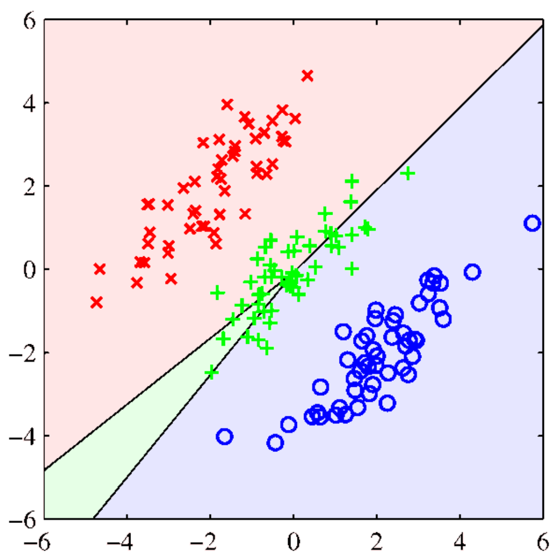
Linear regression: masking problem



One linear discriminant per class: $s_c(\mathbf{x}) = \mathbf{w}_c^T \mathbf{x}$

Nothing ever gets assigned to class 2!

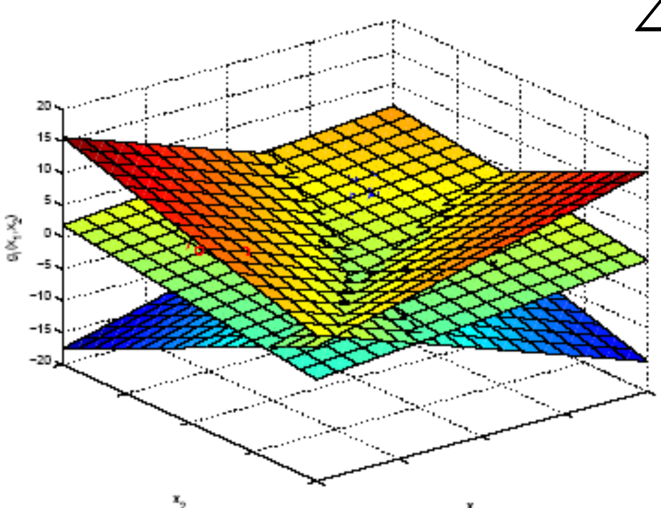
2D version:



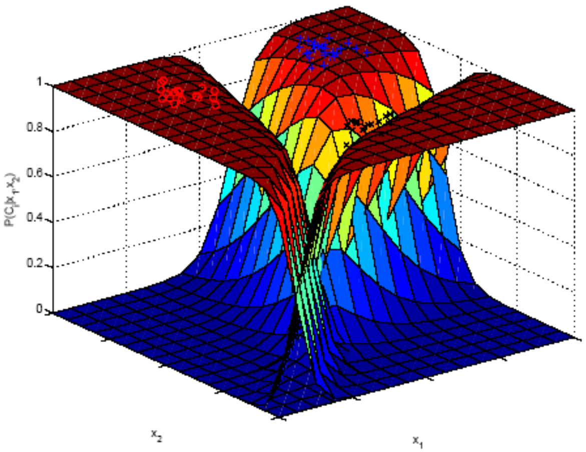
Multiple classes & logistic regression

Soft maximum (softmax) of competing classes:

$$P(y = c|\mathbf{x}; \mathbf{W}) = \frac{\exp(\mathbf{w}_c^T \mathbf{x})}{\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^T \mathbf{x})} \doteq g_c(\mathbf{x}, \mathbf{W})$$



Discriminants (inputs)



Softmax (outputs)

Loss function for single-class classification

Training: given $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$, estimate optimal $\mathbf{w}$

Loss function: quantify appropriateness of $\mathbf{w}$

$$L(S, \mathbf{w}) = -\log P(\mathbf{y}|\mathbf{X}; \mathbf{w})$$

$$= -\sum_{i=1}^{N} y^i \log g(\mathbf{w}^T \mathbf{x}^i) + (1 - y^i) \log(1 - g(\mathbf{w}^T \mathbf{x}^i))$$

Bernoulli model for posterior distribution:

$$P(Y = y|X = \mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T \mathbf{x})^y (1 - g(\mathbf{w}^T \mathbf{x}))^{1-y}$$

Bernoulli & Categorical distribution

Binary random variable $$Y \in \{0, 1\}$$

Bernoulli Distribution:
$$P(Y = c) = \begin{cases} p & c = 1 \\ 1 - p & c = 0 \end{cases}$$
$$= p^c (1 - p)^{1-c}$$

Discrete random variable $$Y \in \{1, \ldots, K\}$$

$$P(Y = c) = \begin{cases} p_1, & c = 1 \\ \vdots & \\ p_K, & c = K \end{cases}$$
$$= \prod_{k=1}^{K} p_k^{[c=k]}$$

(where []: Iverson bracket)

Parameter estimation, multi-class case

One-hot label encoding: $\mathbf{y}^i = (0, 0, 1, 0)$

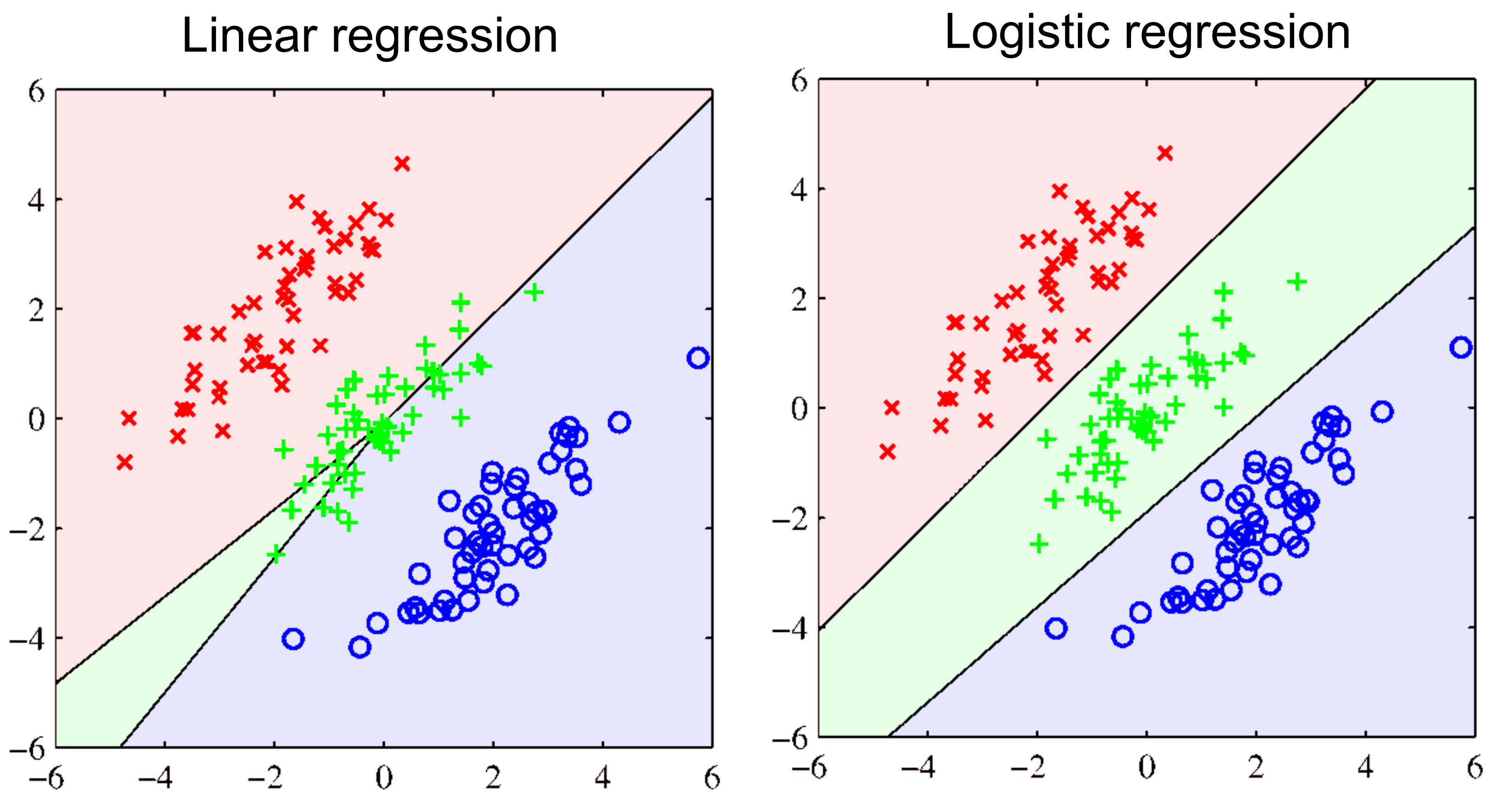
Likelihood of training sample: $(\mathbf{y}^i, \mathbf{x}^i)$

$$P(\mathbf{y}^i | \mathbf{x}^i; \mathbf{w}) = \prod_{c=1}^{C} \left(g_c(\mathbf{x}, \mathbf{W})\right)^{\mathbf{y}_c^i}$$

Optimization criterion:

$$L(\mathbf{W}) = -\sum_{i=1}^{N} \sum_{c=1}^{C} \mathbf{y}_c^i \log\left(g_c(\mathbf{x}, \mathbf{W})\right)$$

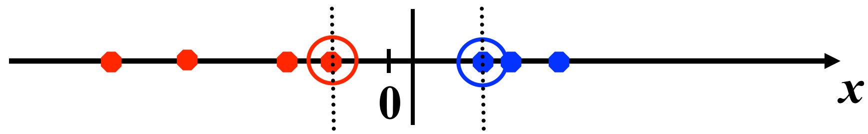
Logistic vs Linear Regression, n>2 classes



Logistic regression does not exhibit the masking problem

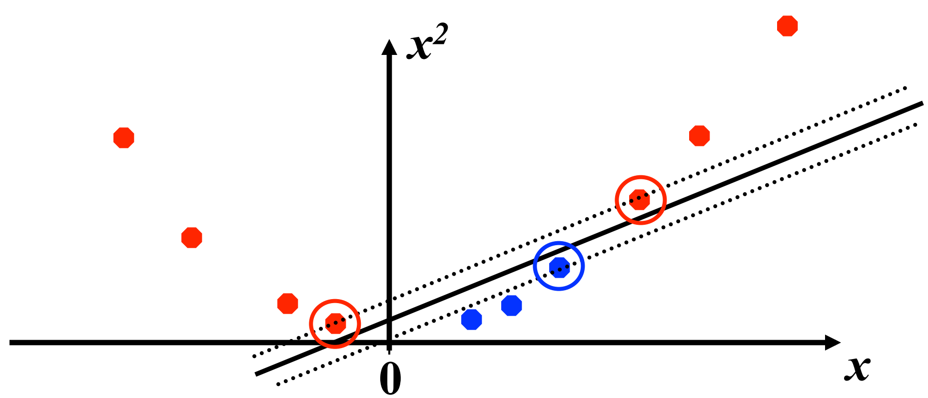
Non-linear detection boundaries

- Datasets that are linearly separable (with some noise) work out great:

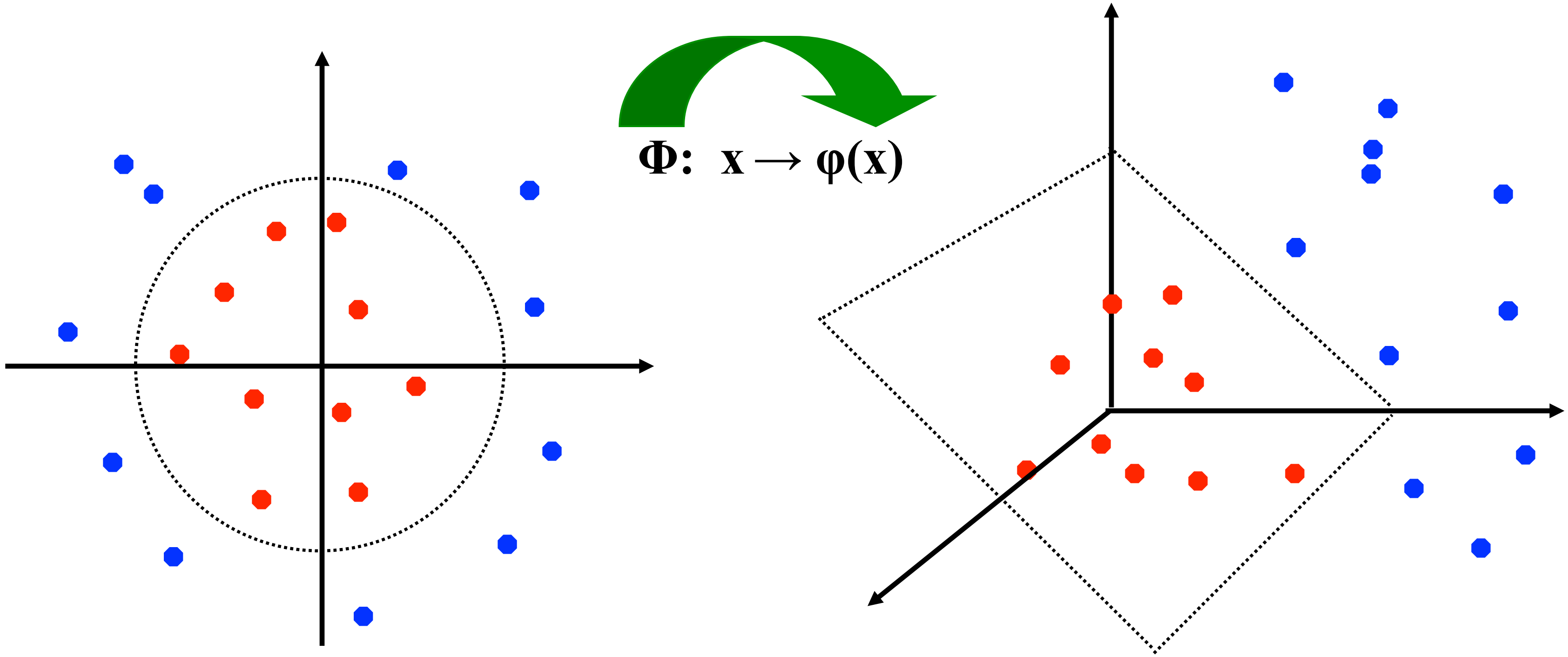


- But what are we going to do if the dataset is just too hard?

- How about … mapping data to a higher-dimensional space:



Non-linear decision boundaries



Parameter estimation, non-linear case

Linear case:

$$L(\mathbf{W}) = -\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbf{y}_c^i \log\left(g_c(\mathbf{x}, \mathbf{W})\right)$$

Nonlinear case:

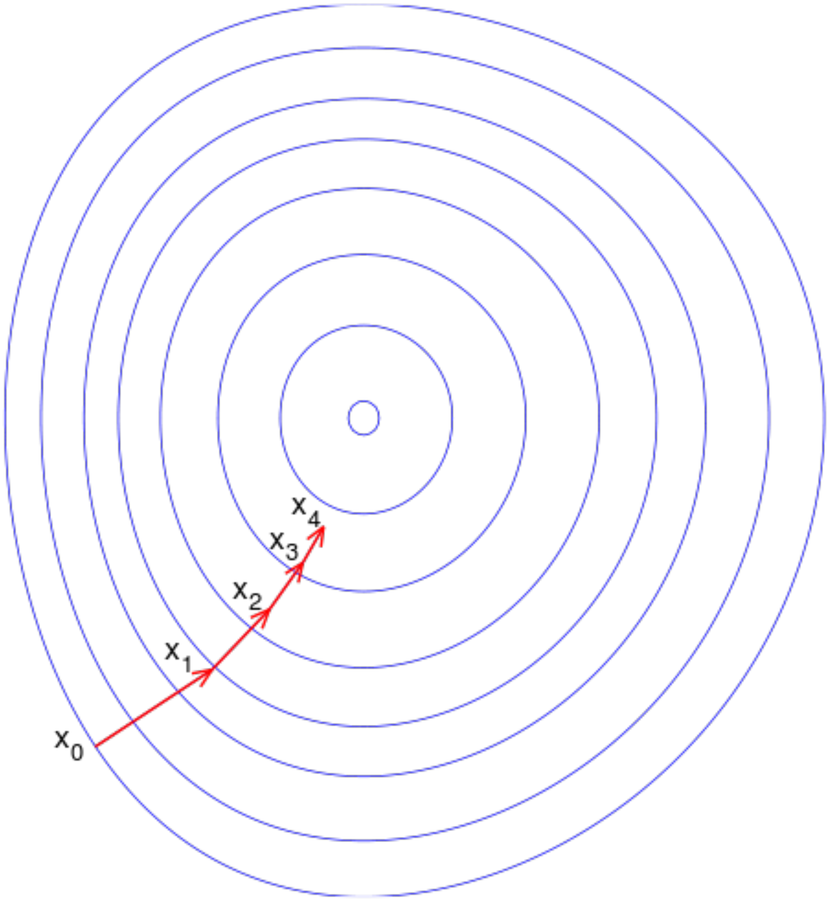
$$L(\mathbf{W}') = -\sum_{i=1}^{N}\sum_{c=1}^{C}\mathbf{y}_c^i \log\left(g_c(\phi(\mathbf{x}), \mathbf{W}')\right)$$

Lecture outline

Recap & problems of linear regression

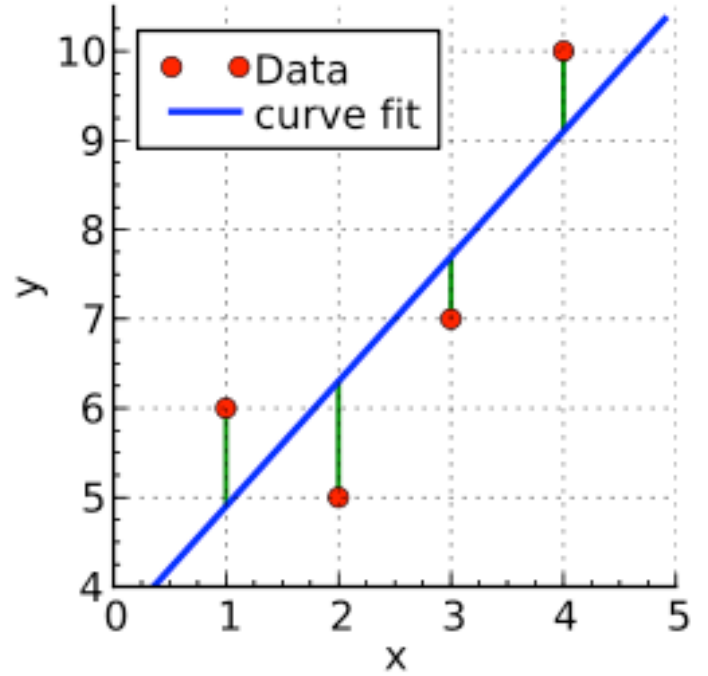
Logistic Regression

- Training criterion formulation
- Interpretation
- Optimization



Recap: Sum of squared errors criterion

$$y^i = \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$



Loss function: sum of squared errors

$$L(\mathbf{w}) = \sum_{i=1}^{N} (\epsilon^i)^2$$

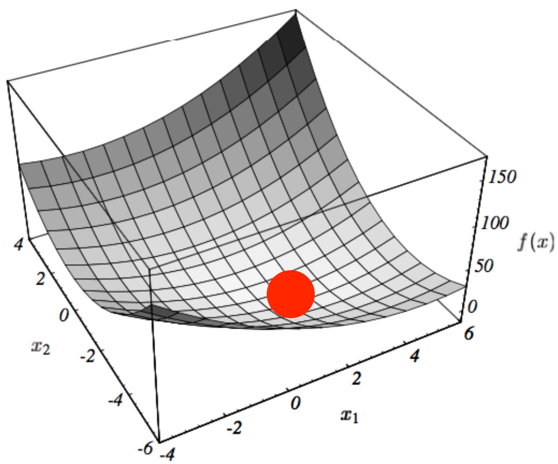
Expressed as a function of two variables:

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2$$

Question: what is the best (or least bad) value of w?

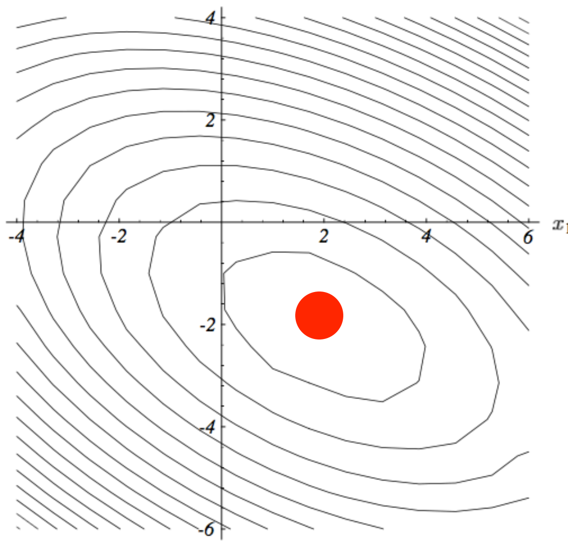
Answer: least squares

Gradient-based optimization



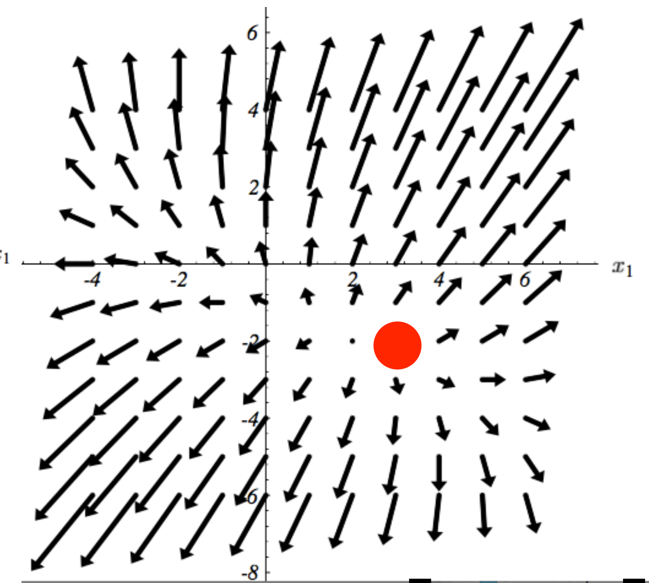
$$f(\mathbf{x})$$

2D function graph



$$f(\mathbf{x}) = c$$

isocontours



$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

gradient field

● **at minimum of function:** $\nabla f(\mathbf{x}) = \mathbf{0}$

Recap: condition for optimum

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = 0 \quad \Leftrightarrow$$

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

$$\frac{\partial L(w_0, w_1)}{\partial w_1} = 0 \quad \Leftrightarrow$$

$$\sum_{i=1}^{N} y^i x_1^i = w_0 \sum_{i=1}^{N} x_0^i x_1^i + w_1 \sum_{i=1}^{N} x_1^i x_1^i$$

2 linear equations, 2 unknowns

Least squares solution, in vector form

$$
\begin{aligned}
L(\mathbf{w}) &= \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \\
&= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w}
\end{aligned}
$$

Condition for minimum:

$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

$$-2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\mathbf{w}^* = \mathbf{0}$$

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

Gradient of cross-entropy los

$$L(\mathbf{w}) = -\sum_{i=1}^{N} y^i \log g(\mathbf{w}^T\mathbf{x}^i) + (1-y^i)\log(1-g(\mathbf{w}^T\mathbf{x}^i))$$

$$\frac{\partial L(\mathbf{w})}{\partial w_k} = -\sum_{i=1}^{N}\left[y^i \frac{1}{g(\mathbf{w}^T\mathbf{x}^i)}\frac{\partial g(\mathbf{w}^T\mathbf{x}^i)}{\partial w_k} + (1-y^i)\frac{1}{1-g(\mathbf{w}^T\mathbf{x}^i)}(-\frac{\partial g(\mathbf{w}^T\mathbf{x}^i)}{\partial w_k})\right]$$

Fact: $g(x) = \frac{1}{1+\exp(-x)} \rightarrow \frac{dg}{dx} = g(x)(1-g(x))$

$$= -\sum_{i=1}^{N}\left[y^i \frac{1}{g(\mathbf{w}^T\mathbf{x}^i)} - (1-y^i)\frac{1}{1-g(\mathbf{w}^T\mathbf{x}^i)}\right] g(\mathbf{w}^T\mathbf{x}^i)(1-g(\mathbf{w}^T\mathbf{x}^i))\frac{\partial \mathbf{w}^T\mathbf{x}^i}{\partial w_k}$$

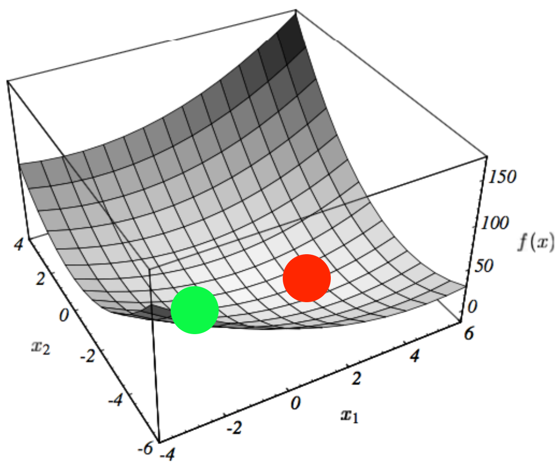
$$= -\sum_{i=1}^{N}\left[y^i(1-g(\mathbf{w}^T\mathbf{x}^i)) - (1-y^i)g(\mathbf{w}^T\mathbf{x}^i)\right] x_k^i$$

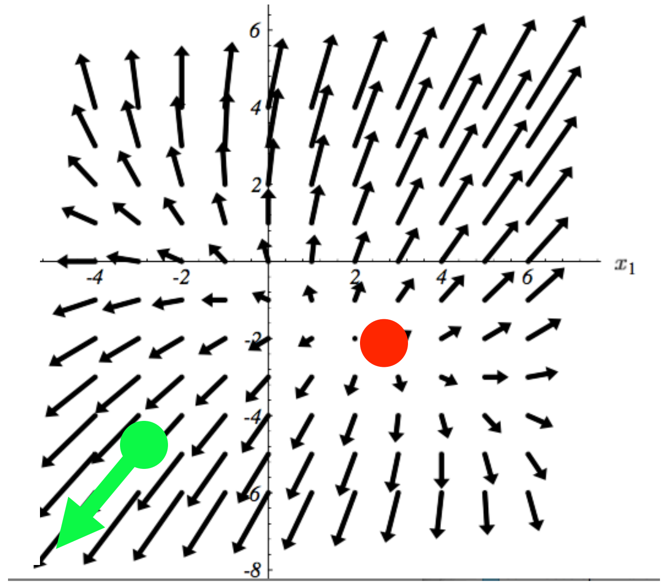
$$= -\sum_{i=1}^{N}\left[y^i - g(\mathbf{w}^T\mathbf{x}^i)\right] \mathbf{x}_k^i$$

$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

Nonlinear system of equations!!

Gradient-based minimization

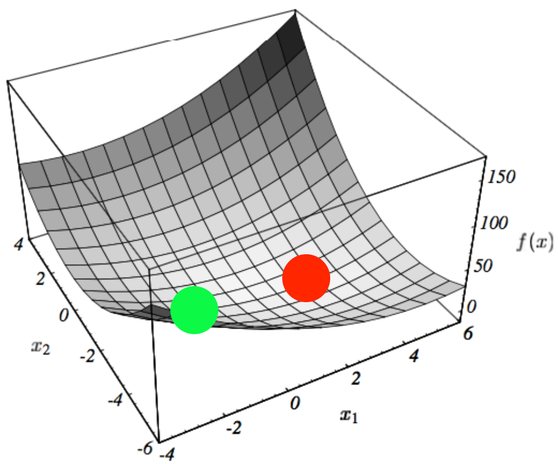


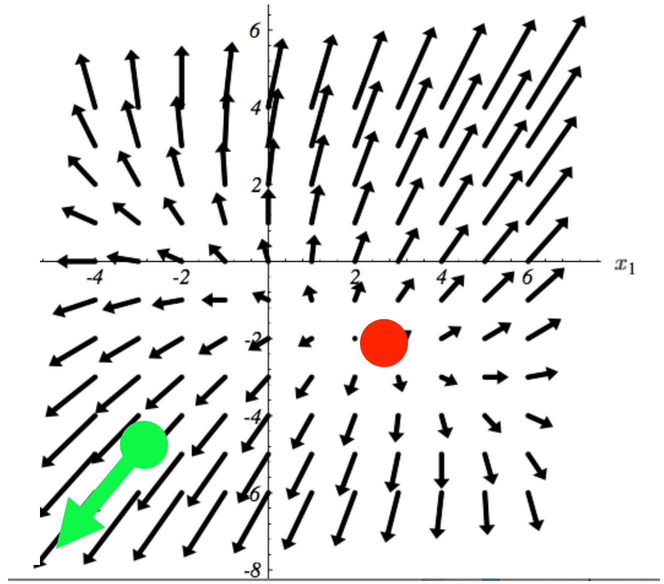


$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Fact: gradient at any point gives direction of fastest increase

Gradient-based minimization





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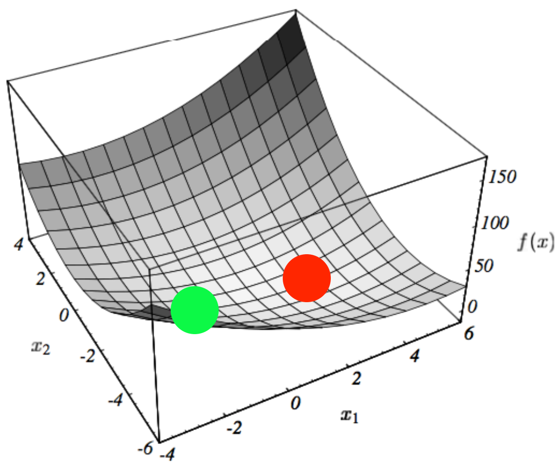
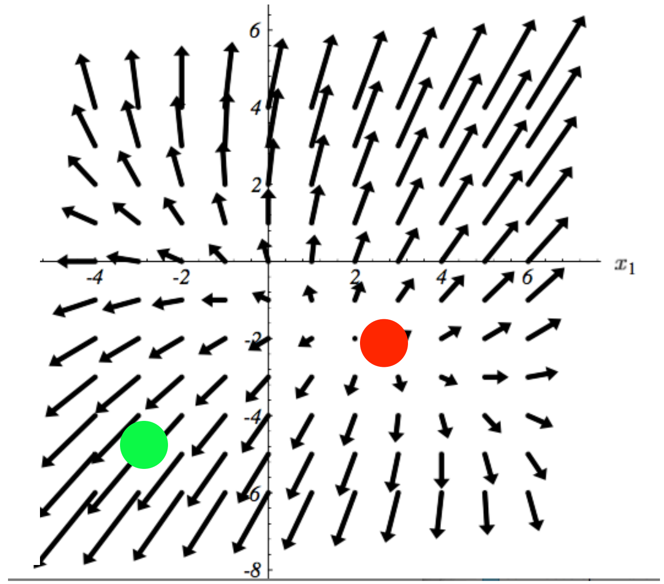
Fact: gradient at any point gives direction of fastest increase

Idea: start at a point and move in the direction opposite to the gradient

Gradient-based minimization





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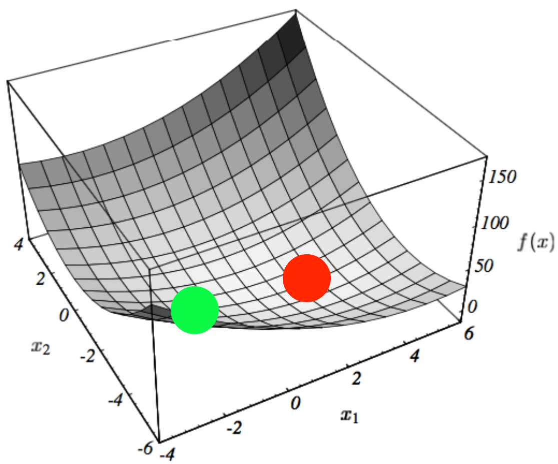

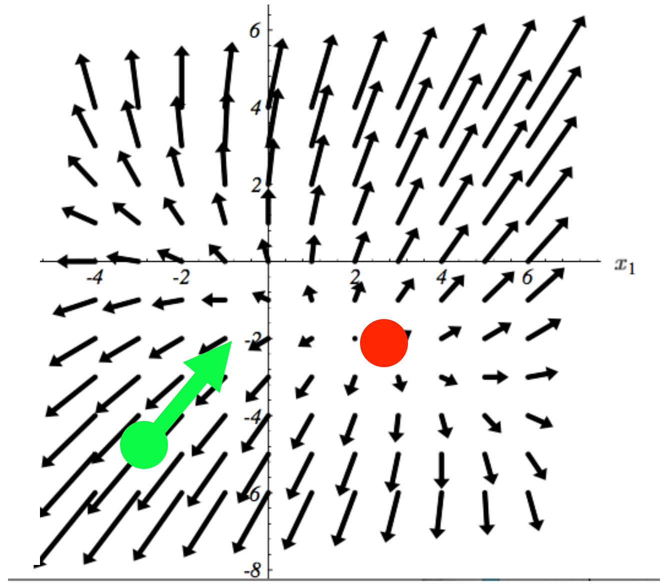

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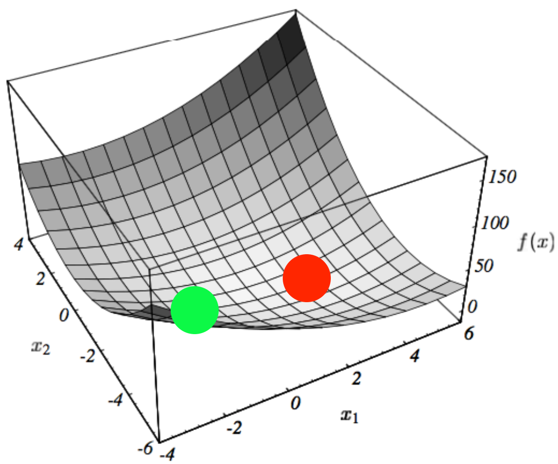
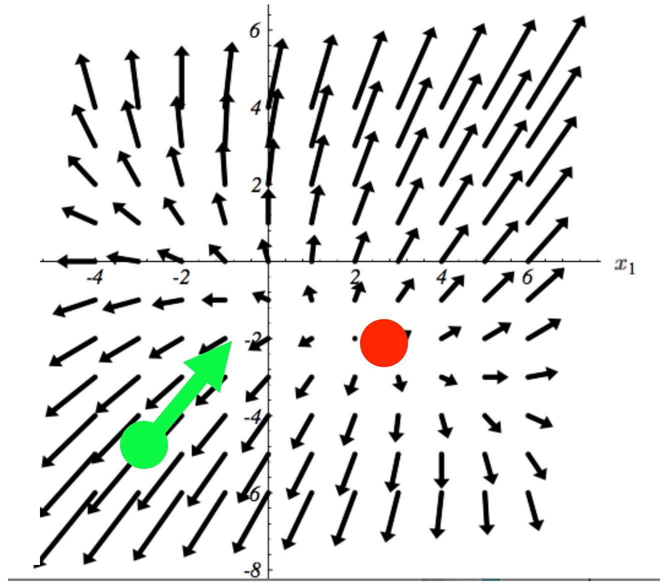
Gradient-based minimization





$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Fact: gradient at any point gives direction of fastest increase

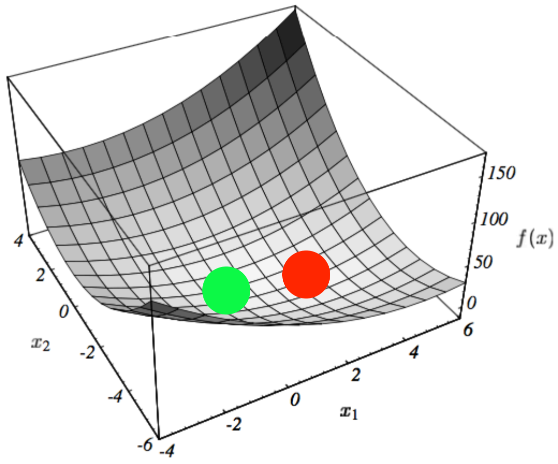
Idea: start at a point and move in the direction opposite to the gradient

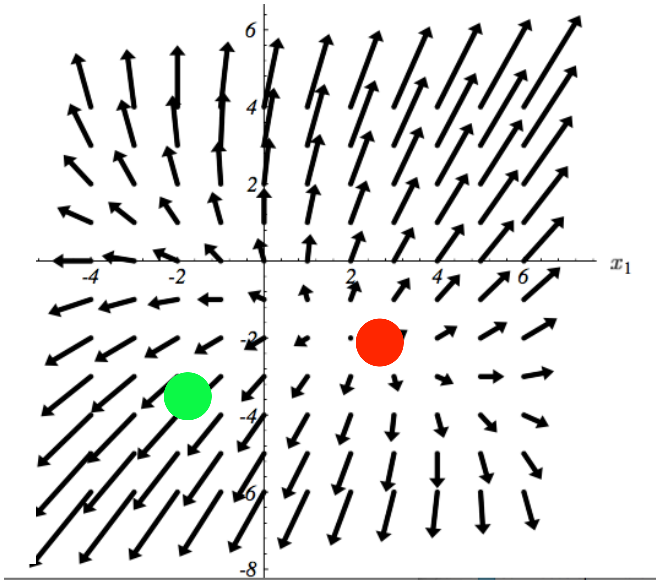
Initialize: $\mathbf{x}_0$

Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$

i=0

Gradient-based minimization

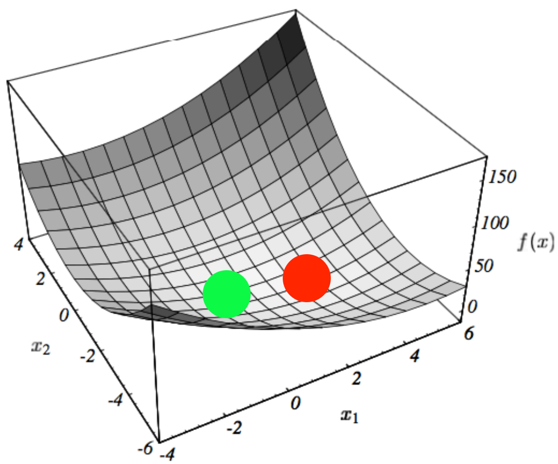


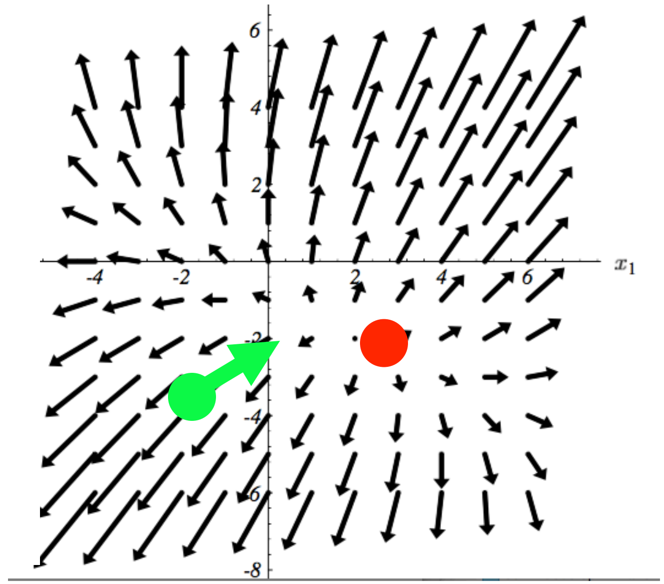


$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Update: $$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$ **i=1**

Gradient-based minimization

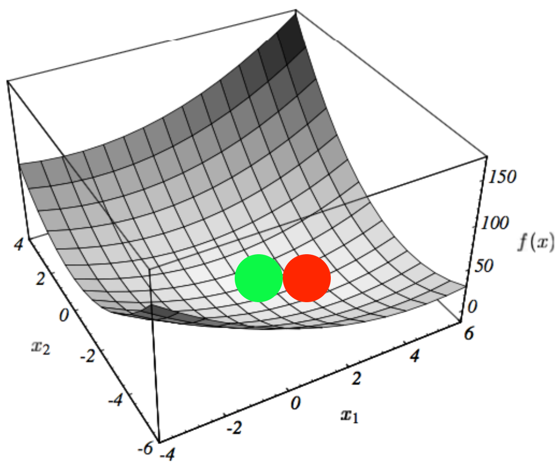


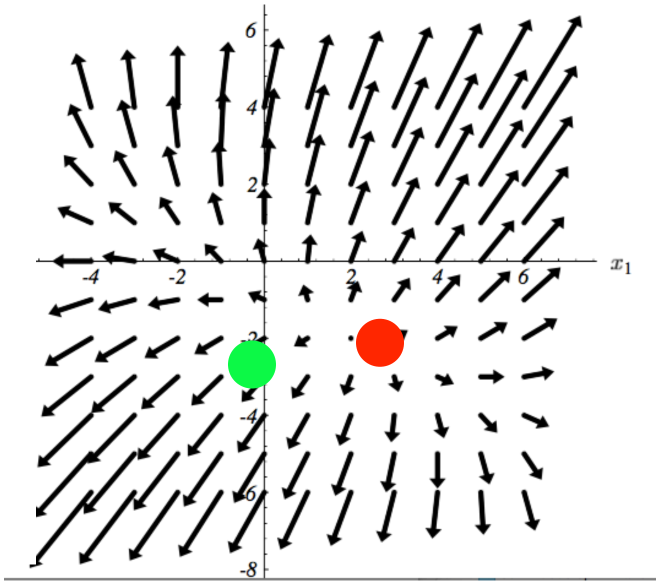


$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Update: $$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$ **i=1**

Gradient-based minimization

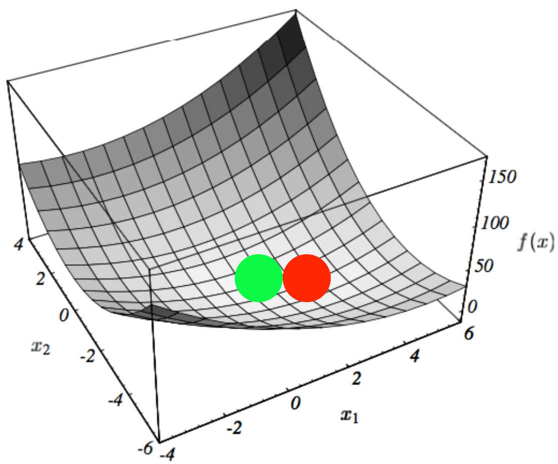


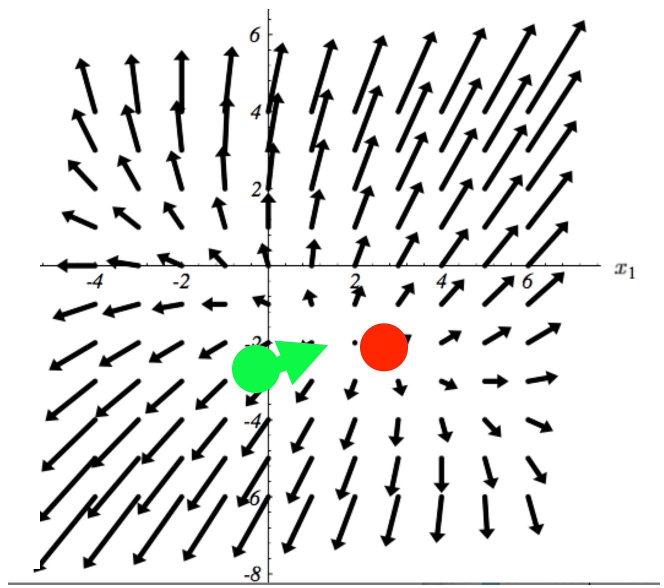


$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$ **i=2**

Gradient-based minimization

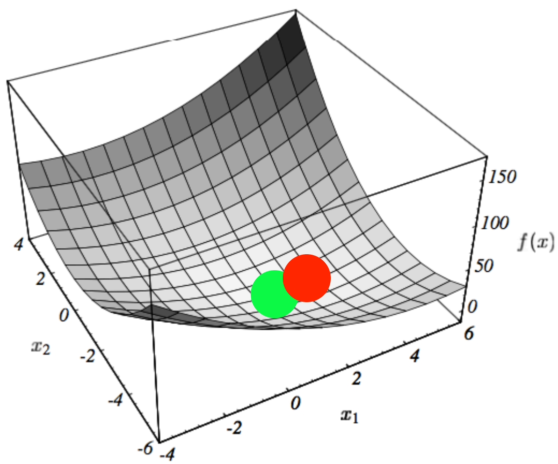


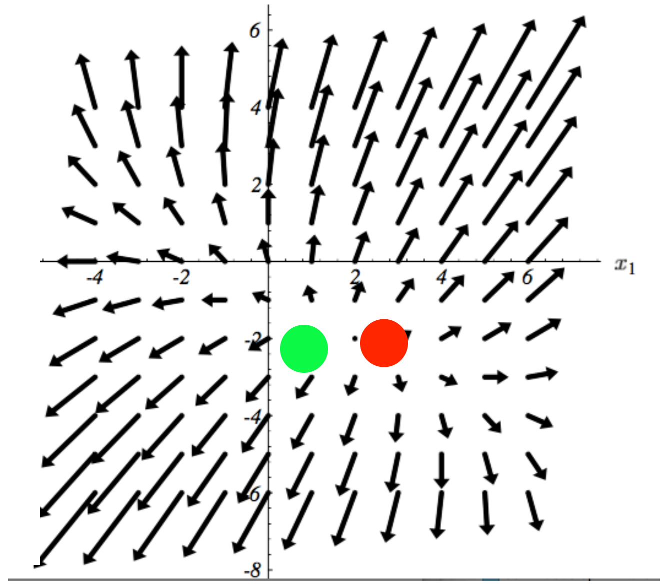


$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Update: $$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$ **i=2**

Gradient-based minimization

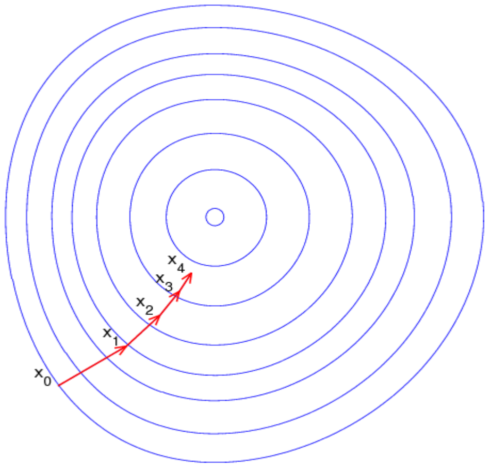




$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

Update: $$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$ **i=3**

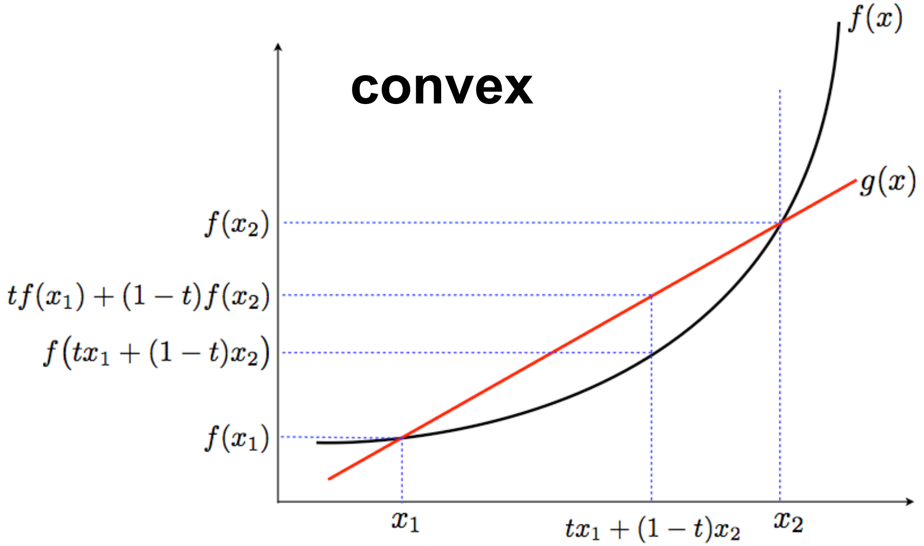
Gradient descent minimization method

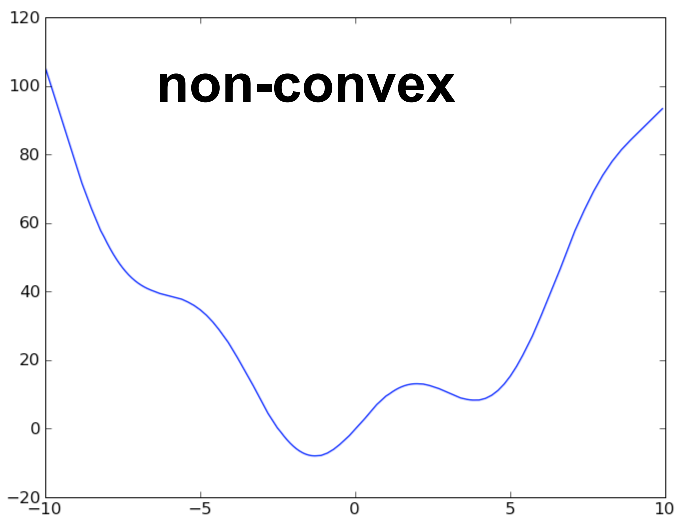


Initialize: $\mathbf{x}_0$

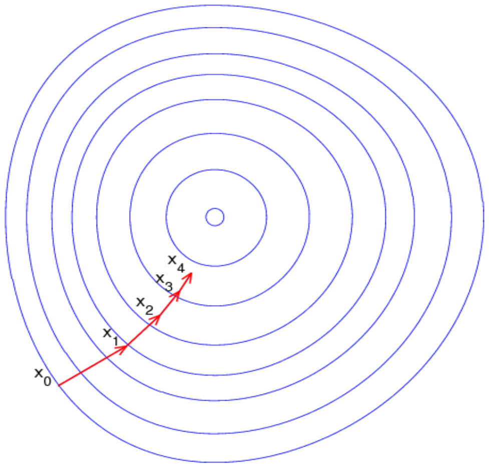
Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$

We can always make it converge for a convex function





Problems of gradient descent



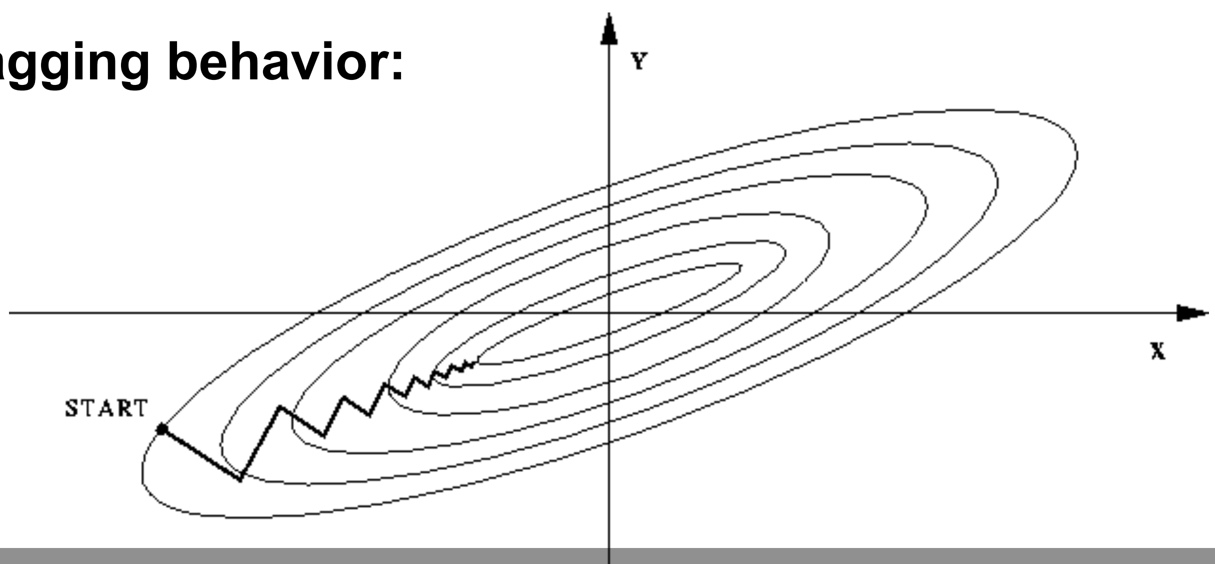
Step-size selection:

Initialize: $\mathbf{x}_0$

Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$

How to set this?

Zig-zagging behavior:



Thought experiment: least squares

Sum of squared errors minimization:

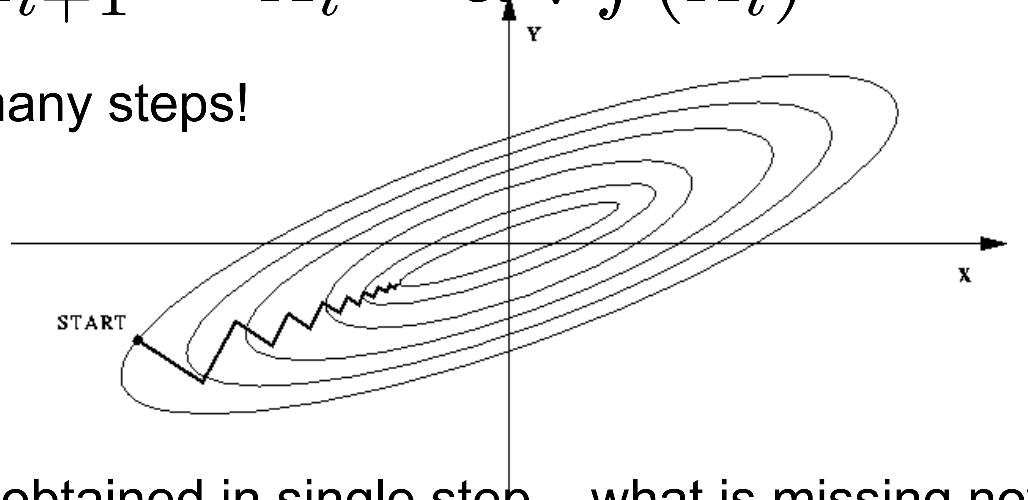
$$f(\mathbf{x}) = (\mathbf{y} - \mathbf{D}\mathbf{x})^T(\mathbf{y} - \mathbf{D}\mathbf{x})$$

Gradient descent:

Initialize: $\mathbf{x}_0$

Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$

May require many steps!



We know solution can be obtained in single step – what is missing now?

Least squares solution, in vector form

$$
\begin{aligned}
L(\mathbf{w}) &= \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \\
&= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w}
\end{aligned}
$$

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

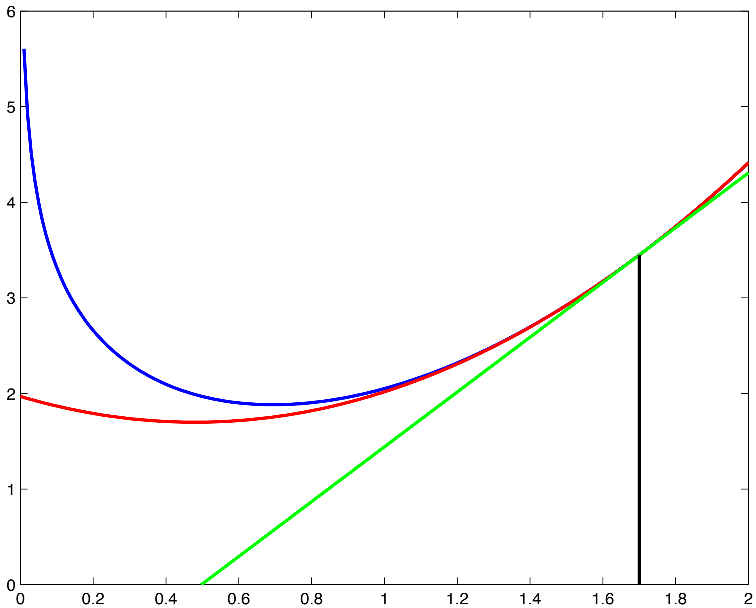
Second-order methods

First- order Taylor series approximation:

$$f(x) \simeq f(a) + (x-a)f'(a) + e(x)$$

Second-order Taylor series approximation:

$$f(x) = f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + e(x)$$



blue:

$$f(x) = x^2 - \log(b) + \exp(\frac{x}{20})$$

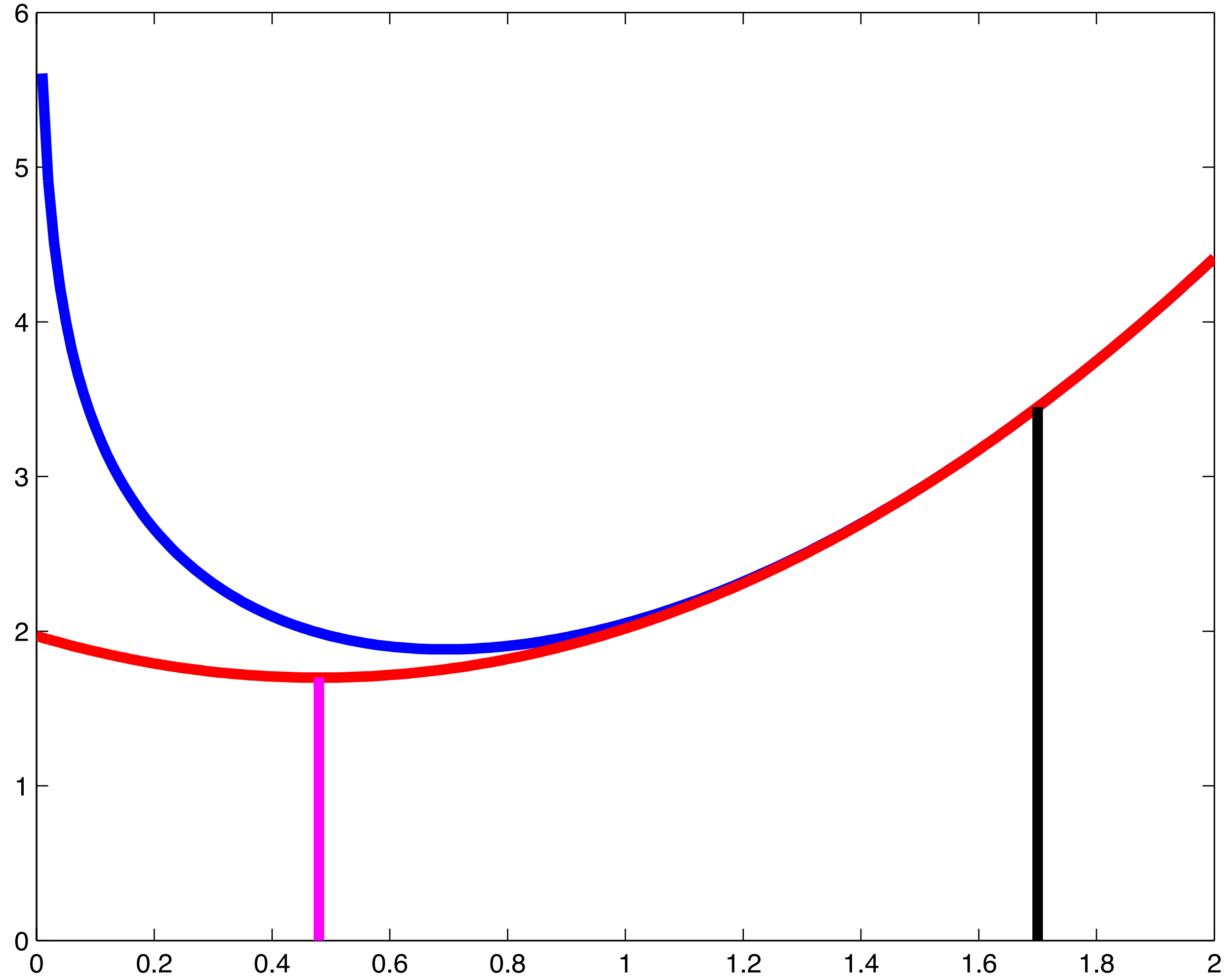
green: linear approximation

$$l(x) = f(a) + (x-a)f'(a)$$

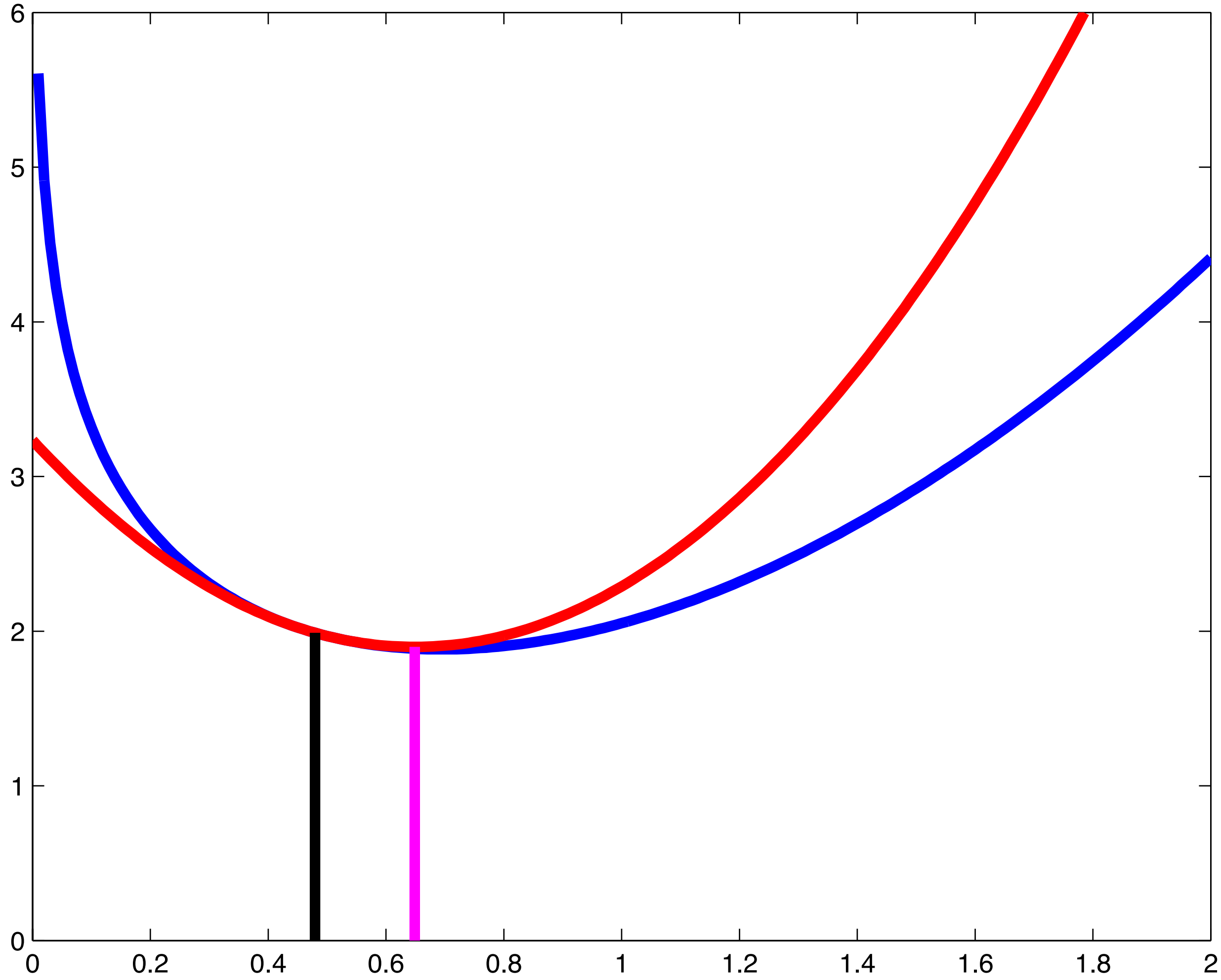
red: quadratic approximation

$$q(x) = f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a)$$

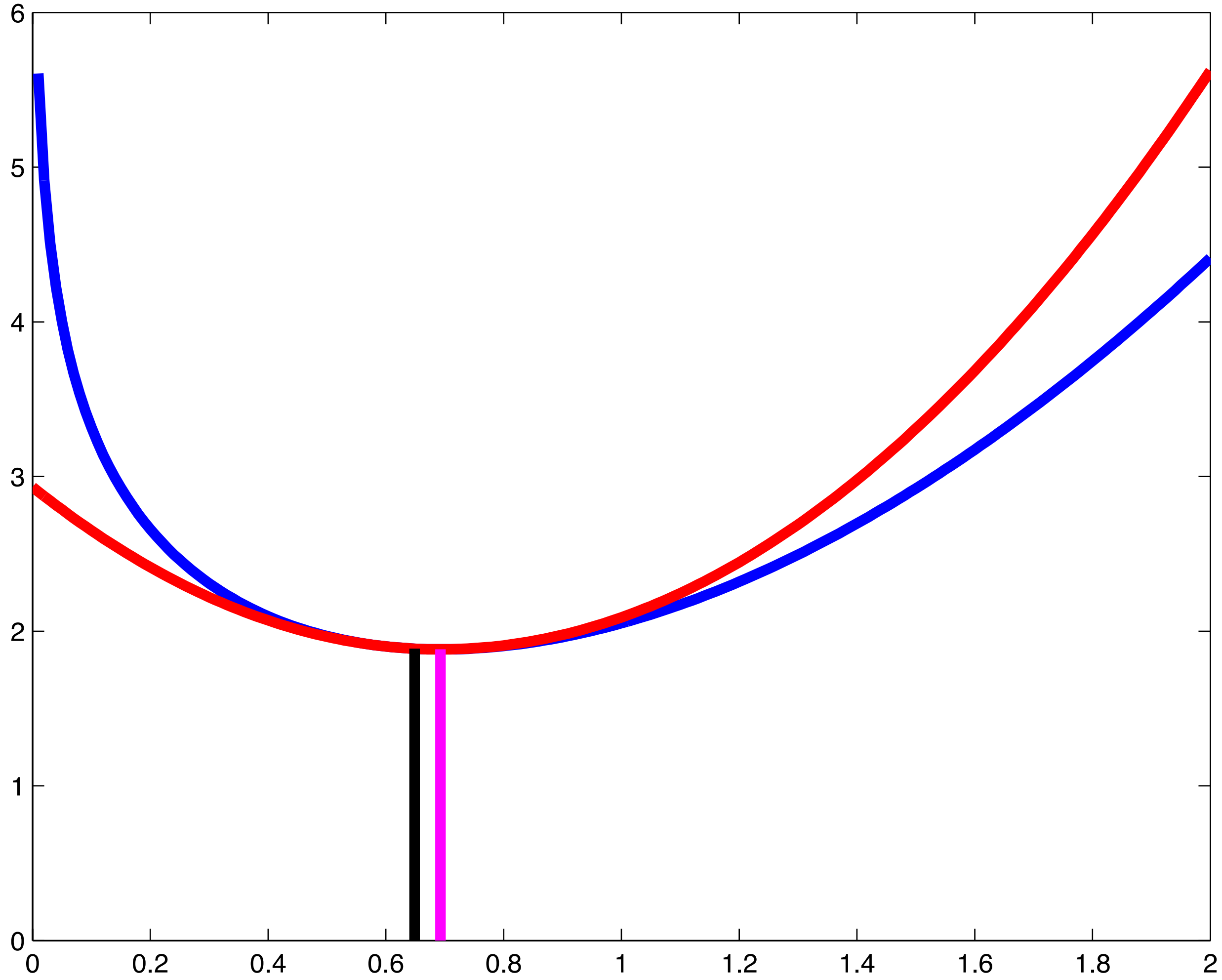
Second-order minimization, 1D



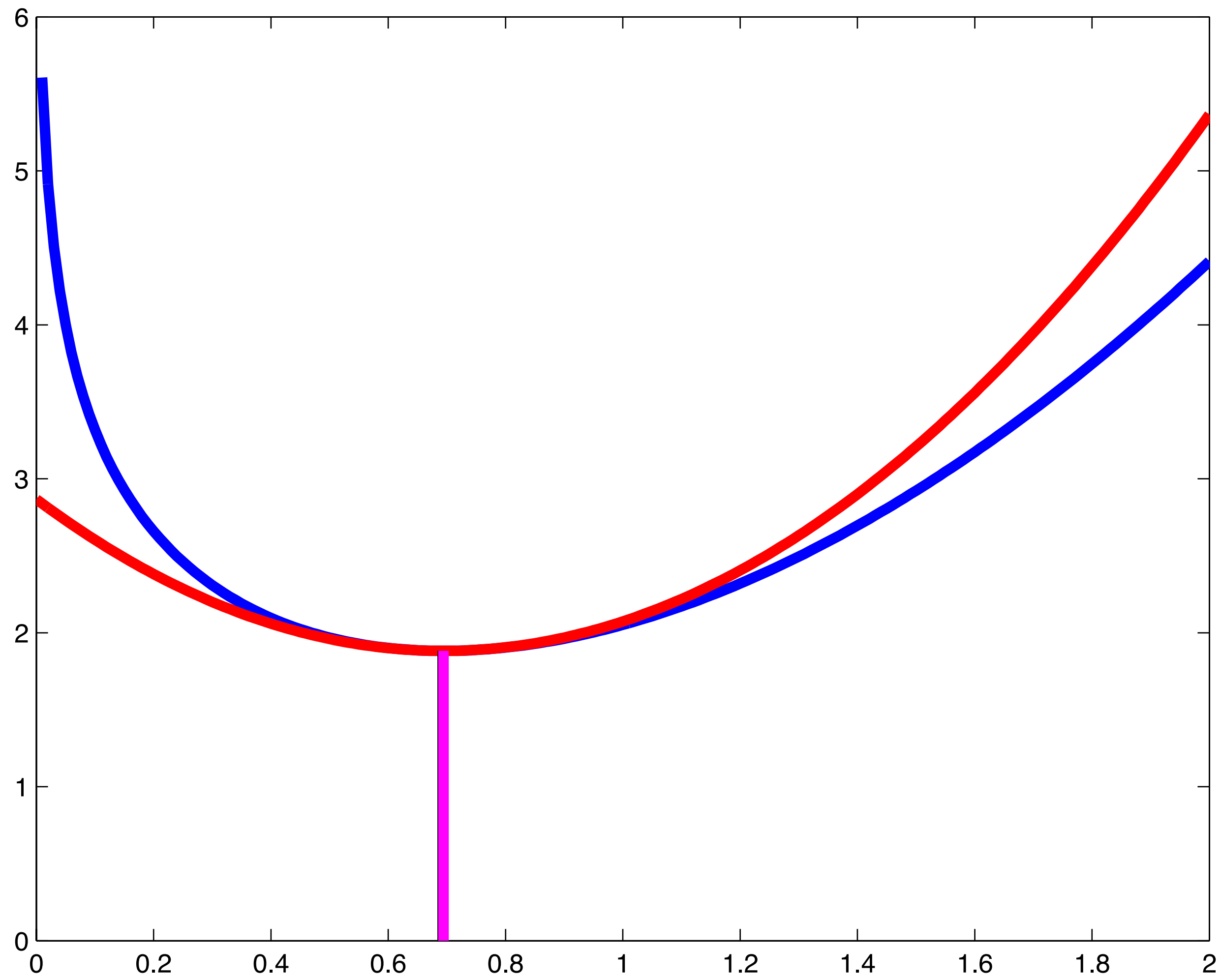
Second-order minimization, 1D



Second-order minimization, 1D



Second-order minimization, 1D



Second-order minimization, 1D

Start from some inititial position, x_0

At any point, form quadratic approximation:

$$f(x) \simeq q(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{1}{2}(x - x_i)^2 f''(x_i)$$

Condition for minimum of quadratic approximation:

$$q'(x) = 0 \rightarrow f'(x_i) + (x - x_i)f''(x_i) = 0$$

Set point in next iteration to be at the minimum of present approximation

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$

Until update is too small

Note: f” sets the update rate α as the inverse of curvature

Second-order methods, multivariate case

First- order Taylor series approximation:

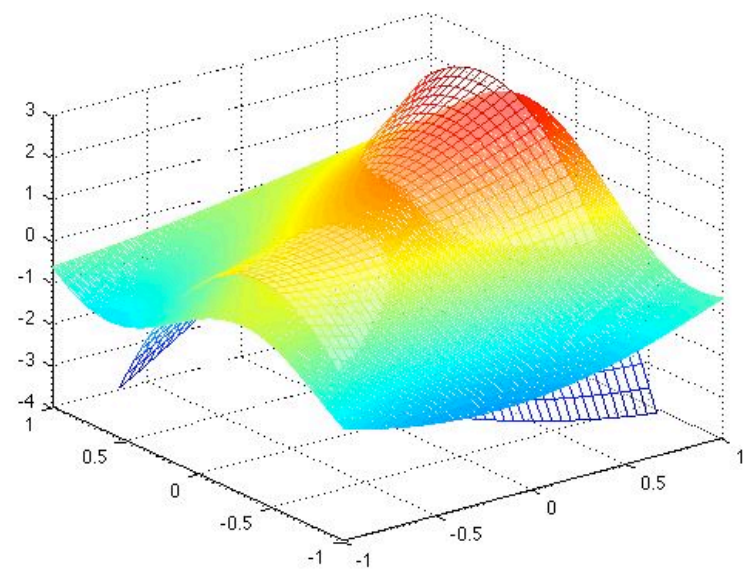
$$f(\mathbf{x}) \simeq f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \nabla f(\mathbf{x}_i)$$

Second-order Taylor series approximation:

$$f(\mathbf{x}) \simeq f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \nabla f(\mathbf{x}_i) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_i)^T \mathbf{H}(\mathbf{x} - \mathbf{x}_i)$$

$$\doteq q(\mathbf{x})$$

$$H_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$



Second-order minimization, 1D

Start from some inititial position, x_0

At any point, form quadratic approximation:

$$f(x) \simeq q(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{1}{2}(x - x_i)^2 f''(x_i)$$

Condition for minimum of quadratic approximation:

$$q'(x) = 0 \rightarrow f'(x_i) + (x - x_i)f''(x_i) = 0$$

Set point in next iteration to be at the minimum of present approximation

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$

Until update is too small

Second-order minimization, N-D (Newton-Raphson)

Start from some inititial position, $\mathbf{x}_0$

At any point, form quadratic approximation:

$$f(\mathbf{x}) \simeq q(\mathbf{x}) = f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \nabla f(\mathbf{x}_i) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_i)^T \mathbf{H}(\mathbf{x}_i)(\mathbf{x} - \mathbf{x}_i)$$

Condition for minimum of quadratic approximation:

$$\nabla q(\mathbf{x}) = 0 \rightarrow \nabla f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \mathbf{H}(\mathbf{x}_i) = 0$$

Set point in next iteration to be at the minimum of present approximation

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (\mathbf{H}(\mathbf{x}_i))^{-1} \nabla f(\mathbf{x}_i)$$

Until update is too small

Newton-Raphson for Logistic Regression

Gradient: $$\frac{\partial L(\mathbf{w})}{\partial w_k} = -\sum_{i=1}^{N} \left[y^i - g(\mathbf{w}^T \mathbf{x}^i) \right] \mathbf{x}_k^i$$

Hessian:

$$\frac{\partial^2 L(\mathbf{w})}{\partial w_k \partial w_j} = \frac{\partial \left(-\sum_{i=1}^{N} \left[y^i - g(\mathbf{w}^T \mathbf{x}^i) \right] \mathbf{x}_k^i \right)}{\partial w_j}$$

$$= \sum_{i=1}^{N} \mathbf{x}_k^i \frac{\partial g(\mathbf{w}^T \mathbf{x}^i)}{\partial w_j} = \sum_{i=1}^{N} \mathbf{x}_k^i g(\mathbf{w}^T \mathbf{x}^i)(1 - g(\mathbf{w}^T \mathbf{x}^i))\mathbf{x}_j^i$$

Summation- and matrix-based expressions

$$H_{k,j} = \frac{\partial^2 L(\mathbf{w})}{\partial w_k \partial w_j} = \sum_{i=1}^{N} \mathbf{x}_k^i g(\mathbf{w}^T \mathbf{x}^i)(1 - g(\mathbf{w}^T \mathbf{x}^i)\mathbf{x}_j^i$$

Matrix version of same result:

$$H(\mathbf{w}) = \mathbf{X}^T \mathbf{R} \mathbf{X}, \quad R_{i,i} = g(\mathbf{w}^T \mathbf{x}^i)(1 - g(\mathbf{w}^T \mathbf{x}^i))$$