

# Lecture 8

## Basics of Optimization

- Gradient Descent, Stochastic Gradient Descent, Newton's Method
- Stochastic Gradient Descent
- Newton's Method
- Example: Solving maximum likelihood estimator for CT imaging

# Contents

*Continuous Optimization*

- Gradient Descent, Stochastic Gradient Descent, Newton's Method
- Stochastic Gradient Descent
- Newton's Method
- Example: Solving maximum likelihood estimator for CT imaging

input, regressor  
 $(y_i, x_{i1}, x_{i2}, \dots, x_{ip})$   
 response

## Multiple linear regression

- set-up:  $p$  variables,  $n$  observations:

$$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} + \epsilon_i, \quad i = 1, \dots, n$$

↑  
intercept.

coefficients  $\beta = [\beta_0, \beta_1, \dots, \beta_p]^T$

column vector.

$$\min_{\beta} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip}))^2$$

least square  
MLE.

- matrix-vector form

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$$

$y = X\beta + \epsilon,$

$$X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{p1} \\ \vdots & \vdots & & \vdots \\ 1 & x_{1n} & \cdots & x_{pn} \end{bmatrix} \in \mathbb{R}^{n \times (p+1)}$$

- parameter estimation

$$\min_{\beta} \|y - X\beta\|_2^2$$

$\|\cdot\|_2$ :  $\ell_2$  norm

$$\|z\|_2 = \sqrt{z^T z}$$

# Simple linear regression

- Linear regression model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad i = 1, 2, \dots, n$$

- To estimate  $(\beta_0, \beta_1)$ , we find values that minimize the sum-of-squares error

$\uparrow$   
intercept
 $\downarrow$   
shape

$$\min_{\beta_0, \beta_1} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \stackrel{\Delta}{=} J(\beta_0, \beta_1)$$

$$\hat{\beta}_1 = S_{xy}/S_{xx}$$

$$\frac{\partial \bar{J}}{\partial \beta_0} = 0 \quad \frac{\partial \bar{J}}{\partial \beta_1} > 0$$

Cross Covariance

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$S_{xy} = \sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x}), \quad S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2$$

Sample Covariance,

$$\begin{aligned} \frac{\partial \bar{J}}{\partial \beta_0} &= \sum_i \frac{\partial \bar{J}}{\partial \beta_0} ( ) \\ &= \sum_i 2(y_i - \beta_0 - \beta_1 x_i)(-1) = 0 \\ \frac{\partial \bar{J}}{\partial \beta_1} &= \sum_i 2(y_i - \beta_0 - \beta_1 x_i)(-x_i) = 0 \end{aligned}$$

$$\Rightarrow \begin{cases} \beta_0 + \beta_1 (\sum_i x_i) = \sum_i y_i \\ (\sum_i x_i) \beta_0 + \beta_1 (\sum_i x_i^2) = \sum_i x_i y_i \end{cases}$$

## Solving multiple linear regression

$$\frac{\partial \hat{y}_i}{\partial x_j} = a_j \quad \frac{\partial a^T x}{\partial x_j} = a_j$$

$$\min_{\beta} f(\beta) := \|y - X\beta\|_2^2, \quad X \in \mathbb{R}^{n \times (p+1)}$$

- Gradient  $\nabla f(\beta) = 2X^T(X\beta - y)$
- Exact solution  $\beta = (X^T X)^{-1} X^T y$
- issue: complexity  $\mathcal{O}(p^3)$   $X^T X \in \mathbb{R}^{(p+1) \times (p+1)}$
- issue:  $(X^T X)^{-1}$  may not be a good idea

$$X = \begin{pmatrix} & & \\ \vdots & \boxed{\phantom{0}} & \dots & \boxed{\phantom{0}} \\ & & \end{pmatrix}$$

↑  
variables

If they're correlated (e.g., predict house price)  
 $X^T X$  is rank-deficient

$$\hat{y}_i$$

$$\|z\|_2^2 = z^T z$$

$$\|y - X\beta\|_2^2$$

$$= y^T y - \beta^T X^T y - y^T X \beta$$

$$+ \beta^T X^T X \beta$$

$$= y^T y - 2\beta^T X^T y + \beta^T X^T X \beta$$

$$\nabla f(\beta) = X^T y - X^T y + \beta^T X^T X \beta$$

# Solving optimization problem

- ▶ solve optimization problem

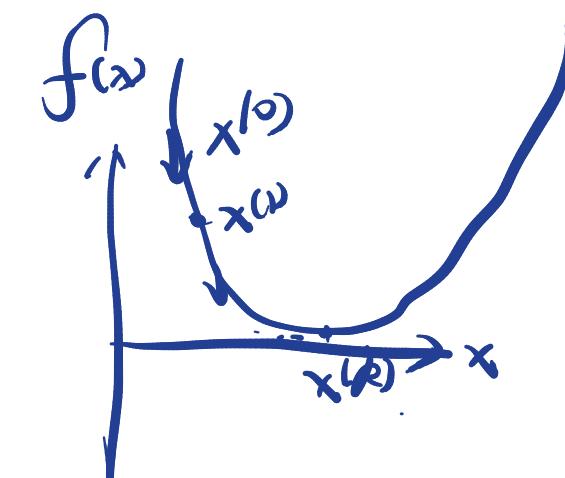
$$\min_x f(x)$$

- ▶ produce sequence of points  $x^{(k)}$ ,  $k = 0, 1, 2, \dots$  with

Initialize  $x^{(0)} \rightarrow x^{(1)} \rightarrow x^{(2)} \rightarrow \dots$ ,  $f(x^{(k)}) \rightarrow p^*$

- ▶ iterative methods for solving optimality condition

$$\nabla f(x^*) = 0$$



approximation algorithm,

## First-order method: Gradient decent

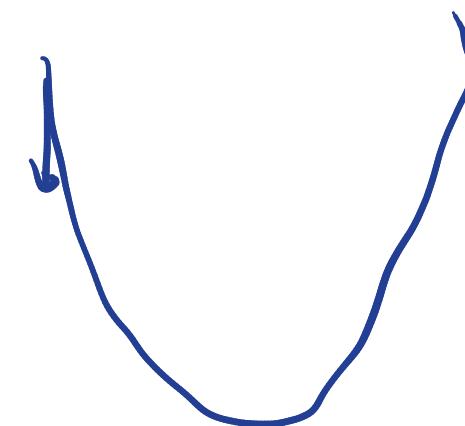
most popular approach.

[MLE, training]  
NN

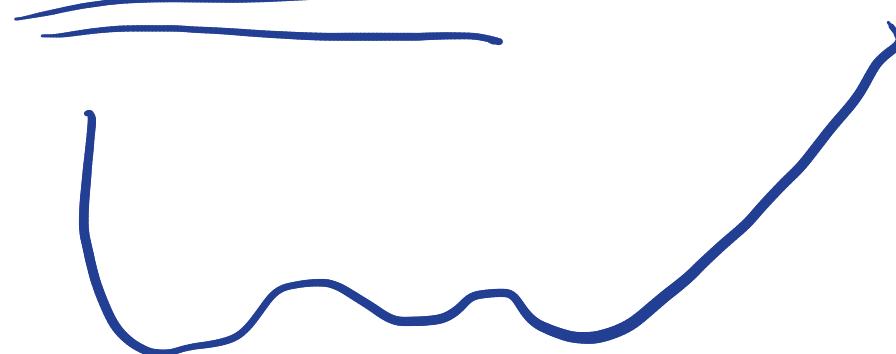
$$x^{(k+1)} = x^{(k)} - t_k \nabla f(x^{(k)})$$

$t_k$ : step-size for the  $k$ th iteration  
 $\nabla f(x)$ : gradient vector

$\min f(x)$



- ▶ for **convex** optimization it gives the global optimum under fairly general conditions.
- ▶ for **nonconvex** optimization it may achieve a local optimum



## Example: solving multiple linear regression

$$\min_{\beta} f(\beta) := \|y - X\beta\|_2^2, \quad X \in \mathbb{R}^{n \times (p+1)}$$

- ▶ Gradient  $\nabla f(\beta) = 2X^\top(X\beta - y)$
- ▶ Exact solution  $\hat{\beta} = (X^\top X)^{-1}X^\top y$ , issue: complexity  $\mathcal{O}(p^3)$
- ▶ Gradient descent

$$\beta^{(k+1)} = \beta^{(k)} - 2t_k X^\top(X\beta^{(k)} - y)$$

no matrix inversion involved

complexity  $\mathcal{O}(np)$

$$= (I - 2t_k X^\top X) \beta^{(k)} + 2t_k X^\top y$$

- ▶ Question: does this converges to the desired result?

matrix

$$\begin{array}{c} \text{square} \\ n_1 \times n_2 \end{array} \quad \begin{array}{c} \text{rectangle} \\ n_2 \times n_3 \end{array}$$

Complexity =  $O(n_1 n_2 n_3)$

## Convex function

A function  $f$  is convex if

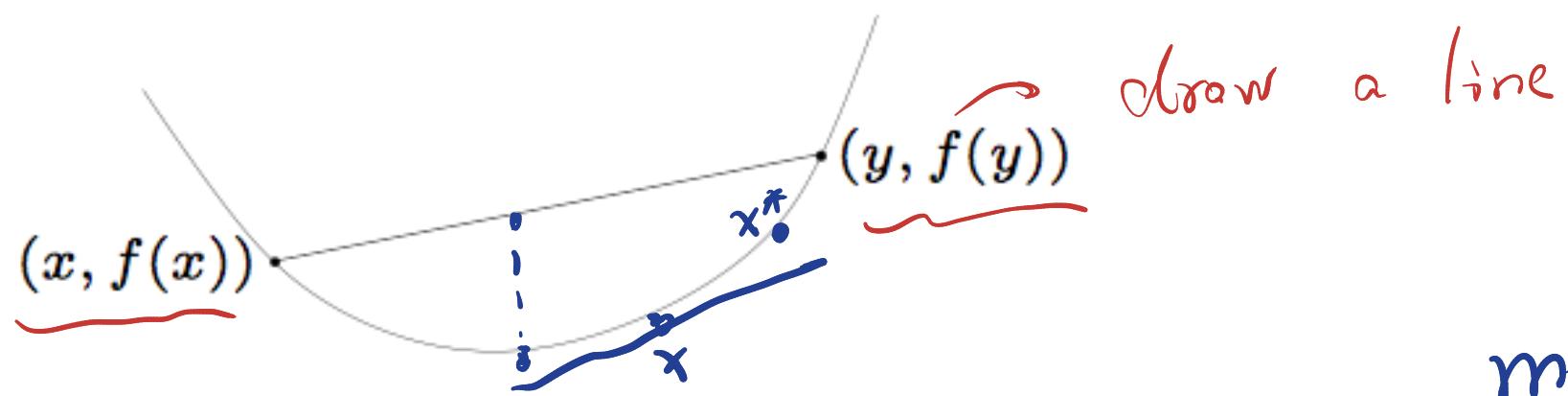
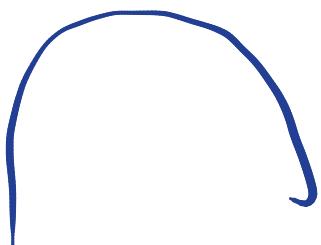
"holds water"

linear interpolation between

$$f(\theta x + (1 - \theta)y) \leq \underbrace{\theta f(x) + (1 - \theta)f(y)}$$

$(x, f(x))$   $(y, f(y))$

• Concave:



Property (first-order):

$$f(x^*) \geq f(x) + g(x)^T(x^* - x)$$

A easy to use way to check: Univariate  $f(x)$  is convex if and only if

$$\frac{\partial^2 f(x)}{\partial x^2} \geq 0$$

$\min f(x)$   
↑  
Convex

⇒ Convex optimization

st.  $x \in S$

$S$ : Convex set

## Convex function

Multivariate  $f(x) : \mathbb{R}^d \rightarrow \mathbb{R}$  is convex if and only if the Hessian matrix is positive semi-definite (PSD)

*Symmetric*

$$H := H[f(x)] = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_d} \\ \cdots & \cdots & \cdots \\ \frac{\partial^2 f(x)}{\partial x_1 \partial x_d} & \cdots & \frac{\partial^2 f(x)}{\partial x_d^2} \end{bmatrix}_{d \times d} \quad H = H^T$$

and this matrix  $H$  is PSD means either one of the following is true

- ✓ 1.  $H$  can be written as  $\underbrace{H = SS^T}$  for some matrix  $S$
- ✓ 2. All eigenvalues of  $H$  are non-negative
- ✓ 3. All the principal sub-matrices of  $H$ , denoted as  $H_i$ , satisfy  $\underbrace{\det(H_i) \geq 0}$

## Example: solving multiple linear regression

- Convex.
- gradient descent.

$$\min_{\beta} \|y - X\beta\|_2^2, \quad X \in \mathbb{R}^{n \times (p+1)}$$

- ▶  $f(\beta) = \|y - X\beta\|_2^2$
- ▶ Gradient  $\nabla f(\beta) = 2X^\top(X\beta - y)$
- ▶ Hessian  $H[f](\beta) = \underbrace{2X^\top X}_{\text{(using basic multivariate calculus)}} = (\sqrt{2}X)^\top(\sqrt{2}X)$

$$\begin{aligned} H[f](\beta) &= \nabla(\nabla f(\beta)) \\ &= 2X^\top X \end{aligned}$$

## Examples

convex functions

► affine:  $ax + b$

► exponential  $e^{ax}$

► powers  $|x|^\alpha$  for  $\alpha \geq 1$

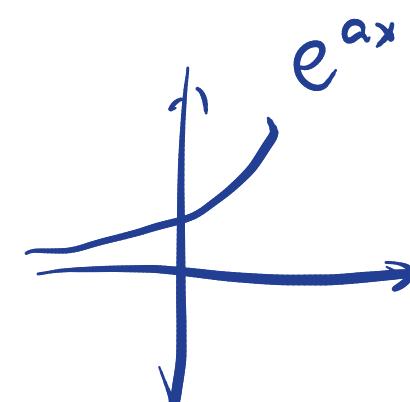
concave:

► affine:  $ax + b$

► log:  $\log x$   $x > 0$

► powers  $x^\alpha$  for  $0 \leq \alpha \leq 1$

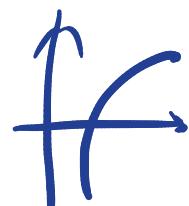
$$f(x) = ax + b$$



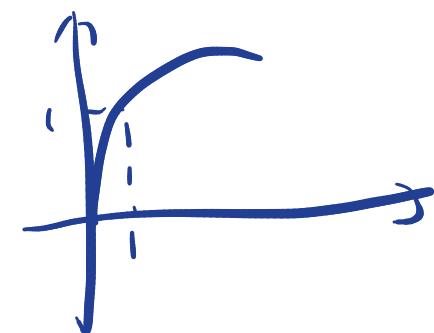
$$\frac{\partial^2}{\partial x^2} f(x) = 0$$

$$f''(x) = \frac{\partial}{\partial x}(a e^{ax}) = a^2 e^{ax} \geq 0$$

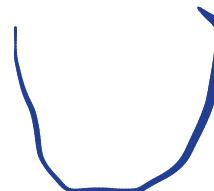
Strictly convex,



$\alpha = \frac{1}{2}$ :



## Convergence results



$$x^* = \arg \min_{x \in \mathbb{R}^n} f(x)$$

- **Gradient descent:** for strongly convex  $f$  with constant  $m$

$$\mathcal{O} \leq f(x^{(k)}) - f(x^*) \leq c^k (f(x^{(0)}) - f(x^*))$$

$\uparrow$   
 $k$ -th iteration      true solution

$c \in (0, 1)$  is a constant depends on  $x^{(0)}$ , step-size,  $m$  etc.

Very simple, but converges very slow.

Number of iterations until  $f(x) - f(x^*) \leq \epsilon$  is  $\mathcal{O}(\log(1/\epsilon))$

$$\begin{aligned} C &= 1/2 \\ C^2 &= 1/4 \\ C^3 &= 1/8 \\ &\vdots \end{aligned}$$

$$\text{if } c^k (f(x^{(0)}) - f(x^*)) \leq \epsilon \Rightarrow k = \mathcal{O}(\log \frac{1}{\epsilon})$$

- **Newton's method:** for strongly convex  $f$  with constant  $m$

number of iterations until  $f(x) - p^* \leq \epsilon$  is  $\mathcal{O}(\log \log(1/\epsilon))$

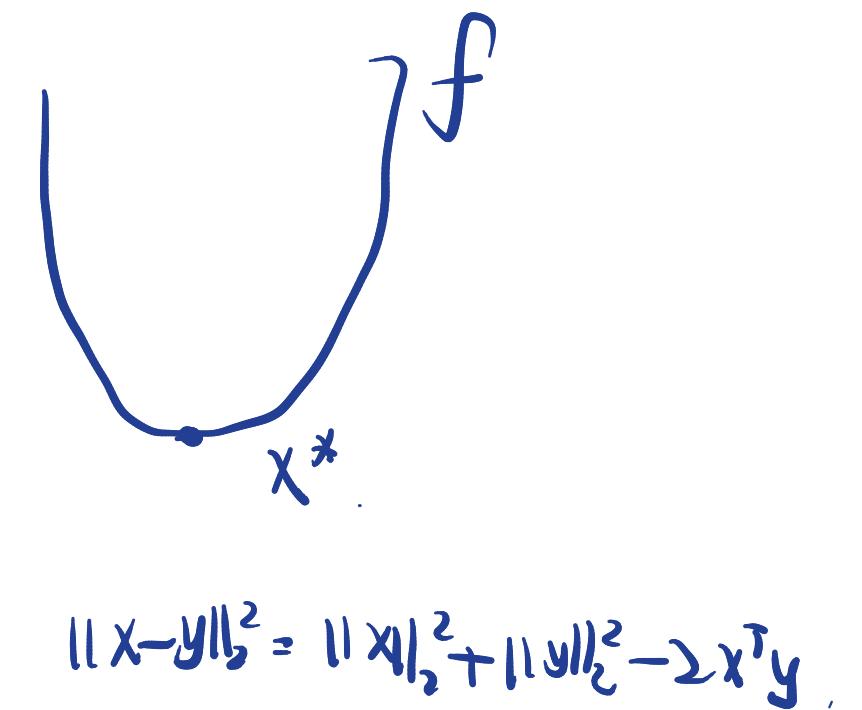
$$\log(10^{10}) = 10$$

$$\log \log(10^{10}) = 1$$

## Convergence proof

**key quantity:** Euclidean distance to the optimal set

Let  $x^*$  be any minimizer of  $f$



$$x^{(k+1)} = x^{(k)} - t_k g^{(k)}$$

$$\begin{aligned} \|x^{(k+1)} - x^*\|_2^2 &= \|x^{(k)} - t_k g^{(k)} - x^*\|_2^2 \\ &= \|x^{(k)} - x^*\|_2^2 - 2t_k g^{(k)T} (x^{(k)} - x^*) + t_k^2 \|g^{(k)}\|_2^2 \\ &\leq \|x^{(k)} - x^*\|_2^2 - 2t_k \underbrace{(f(x^{(k)}) - f^*)}_{f(x^{(k)}) \geq f(x^*) + g^{(k)T}(x^* - x^{(k)})} + t_k^2 \|g^{(k)}\|_2^2 \end{aligned}$$

where  $f^* = f(x^*) \geq f(x^{(k)}) + g^{(k)T}(x^* - x^{(k)})$

Basic inequality: for convex differentiable  $f$ :

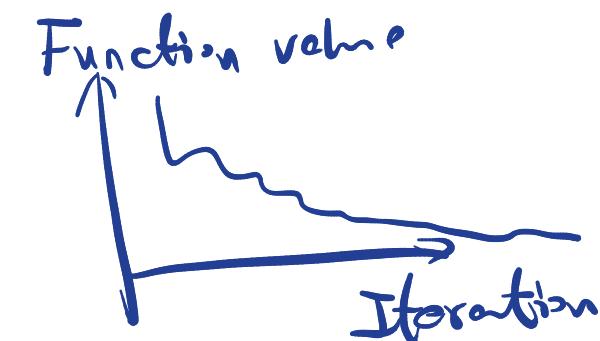
$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$

apply recursively to get

$$\begin{aligned}
& \|x^{(k+1)} - x^*\|_2^2 \\
& \leq \|x^{(1)} - x^*\|_2^2 - 2 \sum_{i=1}^k t_i (f(x^{(i)}) - f^*) + \sum_{i=1}^k t_i^2 \|g^{(i)}\|_2^2 \\
& \quad \text{--- } \mathfrak{S}_{R^2} \text{ --- } \underbrace{\sum_{i=1}^k t_i}_\uparrow (f(x^{(i)}) - f^*) + \underbrace{\sum_{i=1}^k t_i^2 \|g^{(i)}\|_2^2}_\text{--- } \mathfrak{D}_{f(x) = 0} \\
& \leq R^2 - 2 \sum_{i=1}^k t_i (f(x^{(i)}) - f^*) + G^2 \sum_{i=1}^k t_i^2
\end{aligned}$$

# Now use

$$f(x^{(i)}) - f^* \geq f_{\text{best}}^{(k)} - f^*$$



we have

$$f_{\text{best}}^{(k)} - f^* \leq \frac{R^2 + G^2 \sum_{i=1}^k t_i^2}{2 \sum_{i=1}^k t_i}$$

Converge  $\rightarrow c$

$$f_{\text{best}}^{(k)} = \min_{i=1,\dots,k} f(x^{(i)}), \quad \|g\|_2 \leq G \text{ for all gradient } g$$

## Strong convexity and implications

- ▶  $f$  is **strongly convex** on domain  $S$  if there exists an  $m > 0$  such that

$$H[f(x)] \geq mI, \quad \text{for all } x \in S.$$

↓  
identity

if  $H[f(x)] - mI$  is PSD

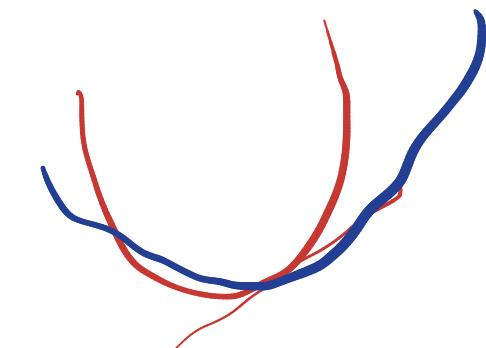
- ▶ **implications**

- ▶ for  $x, y \in S$

$$f(y) \geq f(x) + \nabla f(x)^T(y - x) + \frac{m}{2} \|x - y\|_2^2$$

- ▶ for  $x \in S$ , and  $x^*$  being the minimizer

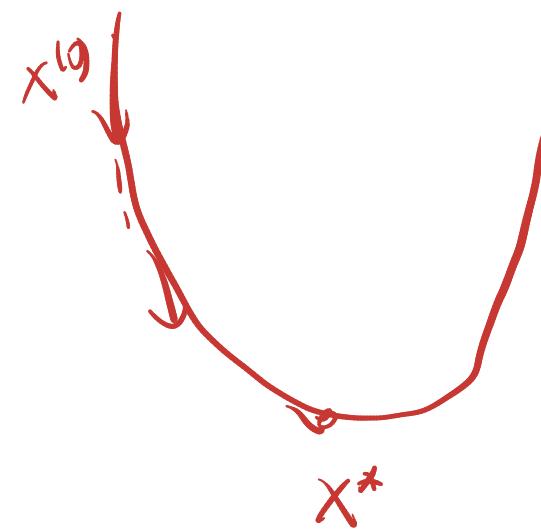
$$f(x) - f(x^*) \leq \frac{1}{2m} \|\nabla f(x)\|_2^2$$



useful as a stopping criterion

## Stopping criterion

- ▶ Stop when  $\frac{R^2 + G^2 \sum_{i=1}^k t_i^2}{2 \sum_{i=1}^k t_i}$  is small
- ▶ Stop when  $\|\nabla f(x)\|_2^2$  is sufficiently small
- ▶ Stop when  $\|x^{k+1} - x^k\|_2$  or  $|f(x^{k+1}) - f(x^k)|$  is small ✓
- ▶ Reality: there isn't a universally good stopping criterion



# Logistic regression

- random variable  $y \in \{0, 1\}$  with distribution

$$h(x; a, b) = \mathbb{P}(y = 1) = \sigma(a^T x + b)$$

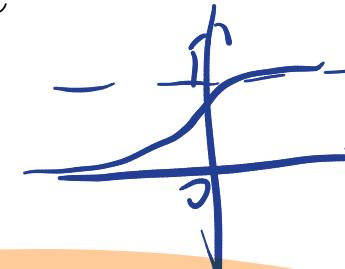
classification  
link function  
variable

Sigmoid function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- maximum likelihood

$$\max_{a, b} \sum_{i=1}^n \{y_i \log h(x_i; a, b) + (1 - y_i) \log(1 - h(x_i; a, b))\}$$



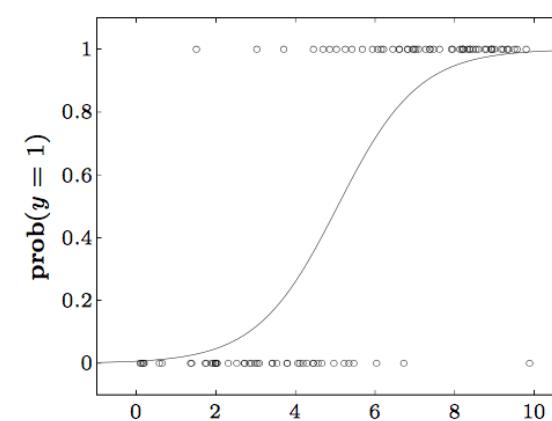
$$\begin{aligned} x \rightarrow -\infty &: \sigma(w) \rightarrow 0 \\ x \rightarrow +\infty &: \sigma(w) \rightarrow 1 \end{aligned}$$

LHW

$$P(y=1) = P$$

$$P(y=0) = 1-P$$

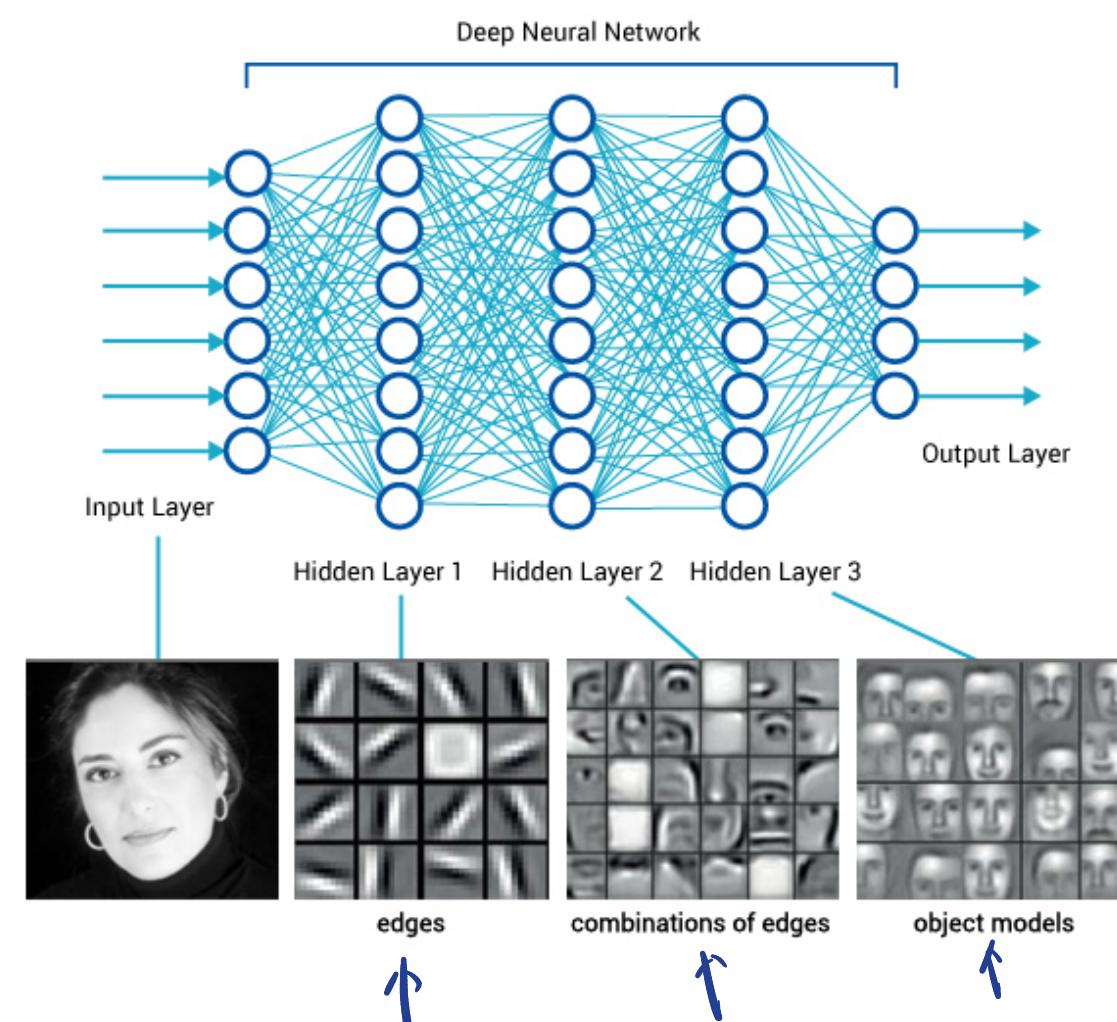
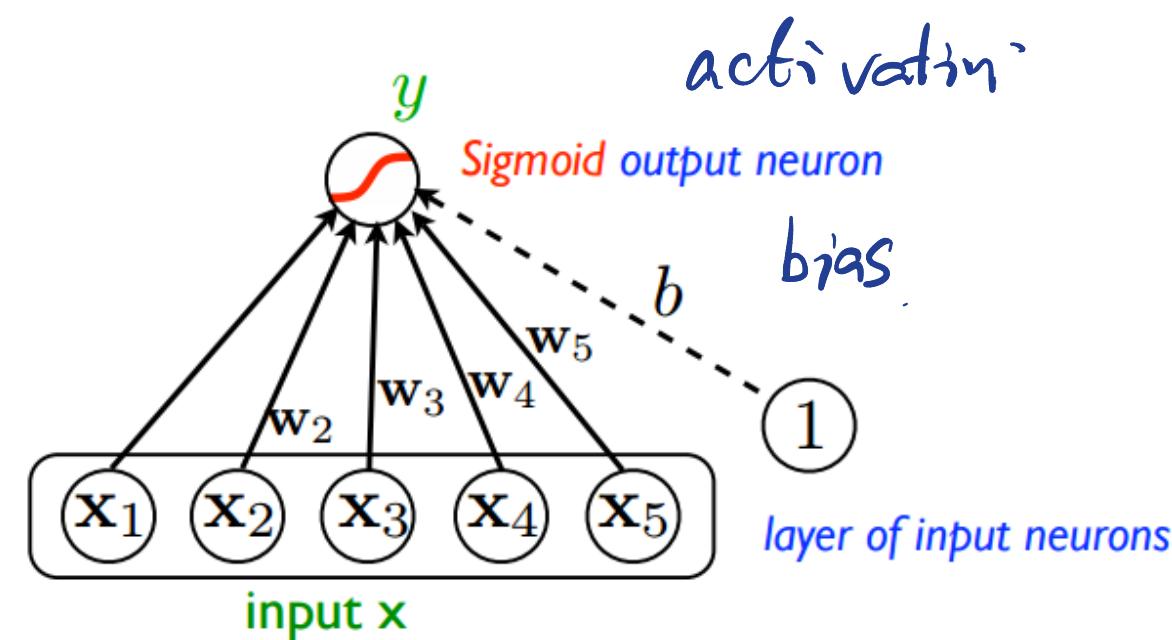
$$\Rightarrow P(Y=\mu) = P^\mu (1-P)^{1-\mu} \quad \mu \in \{0,1\}$$



likelihood function:  
t.r.d. data:  $(x_i, y_i) \in \mathbb{R}^p \downarrow \{0, 1\}$   
 $\Rightarrow \prod_{i=1}^n p^{y_i} (1-p)^{1-y_i}$

$$\begin{aligned} \log \prod_{i=1}^n p^{y_i} (1-p)^{1-y_i} &= \sum_{i=1}^n \log p^{y_i} (1-p)^{1-y_i} = \sum_{i=1}^n y_i \log p + (1-y_i) \log(1-p) \end{aligned}$$

# Deep learning and neural networks



## Example: Optimization in training neural networks

Data:  $(x_i, y_i)$ ,  $i = 1, \dots, n$ .

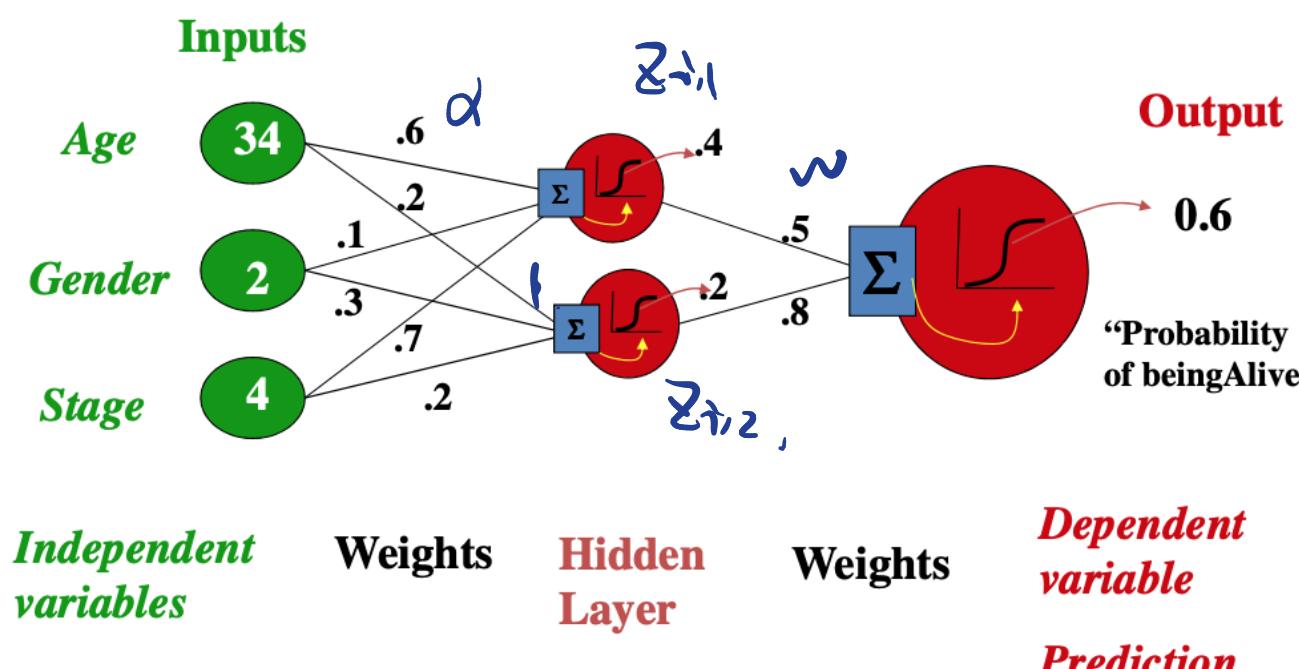
$$\text{Loss function: } \ell(w, \alpha, \beta) = \sum_{i=1}^n (\underbrace{y_i - \sigma(w^T z_i)}_{\min_{w, \alpha, \beta} \ell(w, \alpha, \beta)})^2$$

where

$$z_{i,1} = \sigma(\alpha^T x_i), \quad z_{i,2} = \sigma(\beta^T x_i)$$

Sigmoid function  $\sigma(x) = \frac{1}{1+e^{-u}}$

- ▶ Not a convex objective function
- ▶ Use gradient descent to find a local optimum solution



## Gradient descent: backpropagation

[Pytorch, Tensorflow]

Backpropagation computes the gradient in weight space of a feedforward neural network, with respect to a loss function.

- ▶ Loss function:  $\ell(w, \alpha, \beta) = \sum_{i=1}^n (y_i - \sigma(w^T z_i))^2$
- ▶ Gradient with respect to the weights  $w$  in the last layer (HW).

$$\frac{\partial \ell(w, \alpha, \beta)}{\partial w} = - \sum_{i=1}^n 2(y_i - \sigma(u_i))\sigma(u_i)(1 - \sigma(u_i))z_i$$

where  $u_i = w^T z_i$ ,  $z_{i,1} = \sigma(\alpha^T x_i)$ ,  $z_{i,2} = \sigma(\beta^T x_i)$

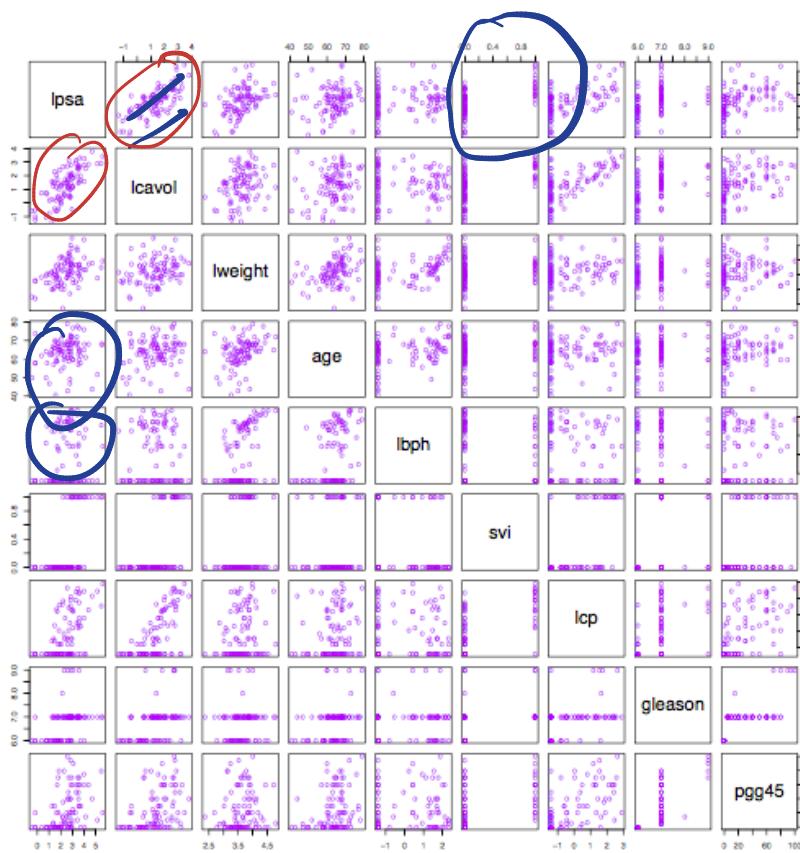
- ▶ Use chain rule, gradient with respect to weights in previous layer

$$\begin{aligned} \frac{\partial \ell(w, \alpha, \beta)}{\partial \alpha} &= \frac{\partial \ell(w, \alpha, \beta)}{\partial z_{i,1}} \frac{\partial z_{i,1}}{\partial \alpha} \\ &= - \sum_{i=1}^n 2(y_i - \sigma(u_i))\sigma(u_i)(1 - \sigma(u_i))w_1\sigma(v_i)(1 - \sigma(v_i))x_i \end{aligned}$$

where  $v_i = \alpha^T x_i$

## Example: prostate cancer

The data for this example come from a study by Stamey et al. (1989). They examined the correlation between the level of prostate-specific antigen and a number of clinical measures in men who were about to receive a radical prostatectomy. The variables are log cancer volume (1cavol), log prostate weight (lweight), age, log of the amount of benign prostatic hyperplasia (1bph), seminal vesicle invasion (svi), log of capsular penetration (1cp), Gleason score (gleason), and percent of Gleason scores 4 or 5 (pgg45). The correlation matrix of the predictors given in Table 3.1 shows many strong correlations. Figure 1.1 (page 3) of Chapter 1 is a scatterplot matrix showing every pairwise plot between the variables. We see that svi is a binary variable, and gleason is an ordered categorical variable. We see, for example, that both 1cavol and 1cp show a strong relationship with the response 1psa, and with each other. We need to fit the effects jointly to untangle the relationships between the predictors and the response.



Scatter plot

FIGURE 1.1. Scatterplot matrix of the prostate cancer data. The first row shows the response against each of the predictors in turn. Two of the predictors, svi and gleason, are categorical.

Variable selection: for multiple linear regression, select the “most important” variables that are responsible for the output:

Lasso (1996)

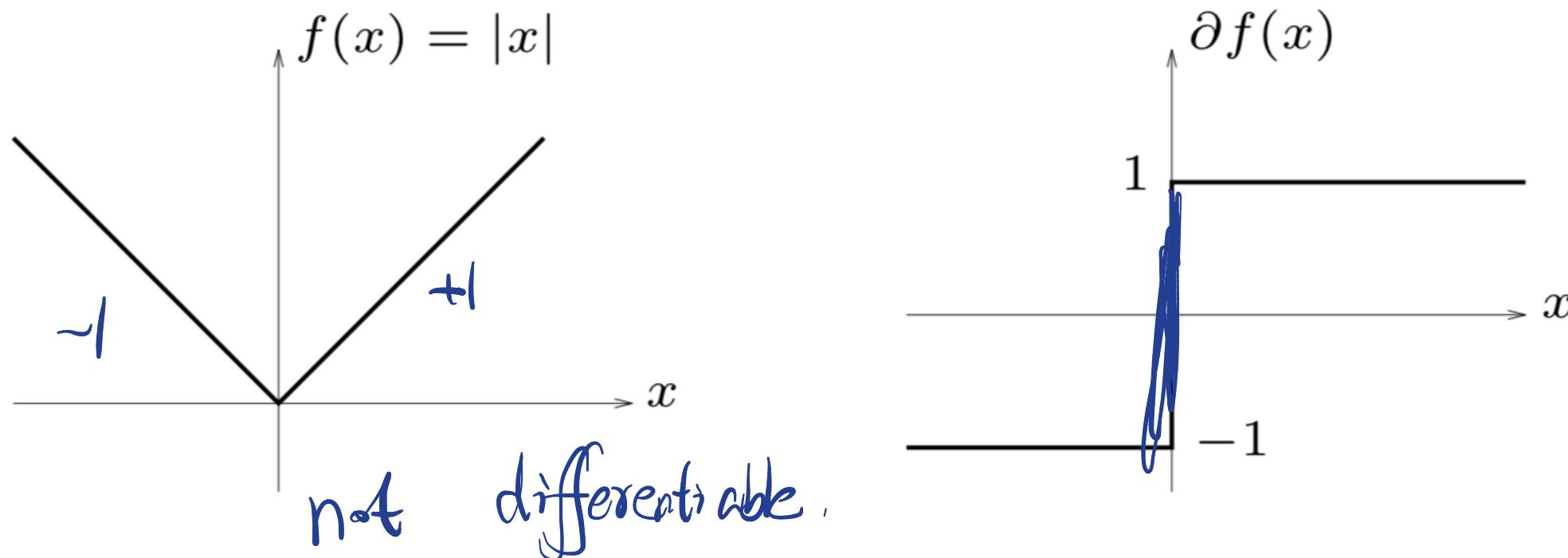
$$\min_{\beta} \|y - X\beta\|_2^2 + \underbrace{\lambda \|\beta\|_1}_{\text{regularizer}}$$

where  $\|\beta\|_1 = \sum_{i=1}^p |\beta_i|$

$\lambda > 0$ : Regularize parameter

## Example of subgradient

$$f(x) = |x|$$



righthand plot shows  $\bigcup \{(x, g) \mid x \in \mathbb{R}, g \in \partial f(x)\}$

We need this to solve lasso:

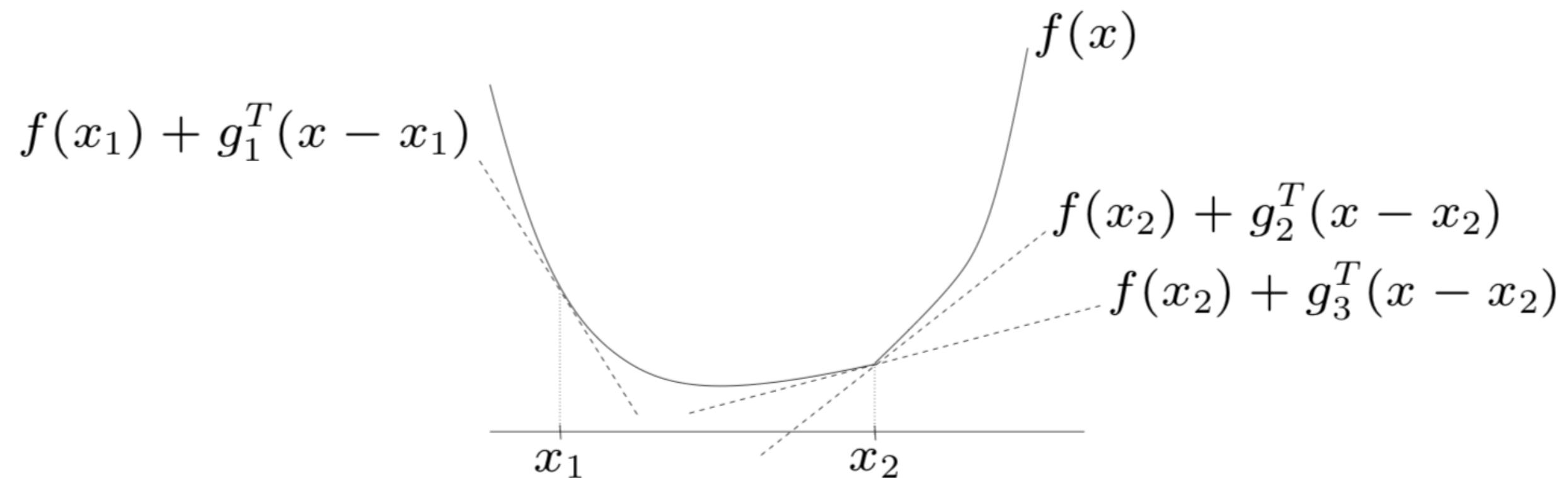
$$\min_{\beta} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

where  $\|\beta\|_1 = \sum_{i=1}^p |\beta_i|$

## Extension: Subgradient

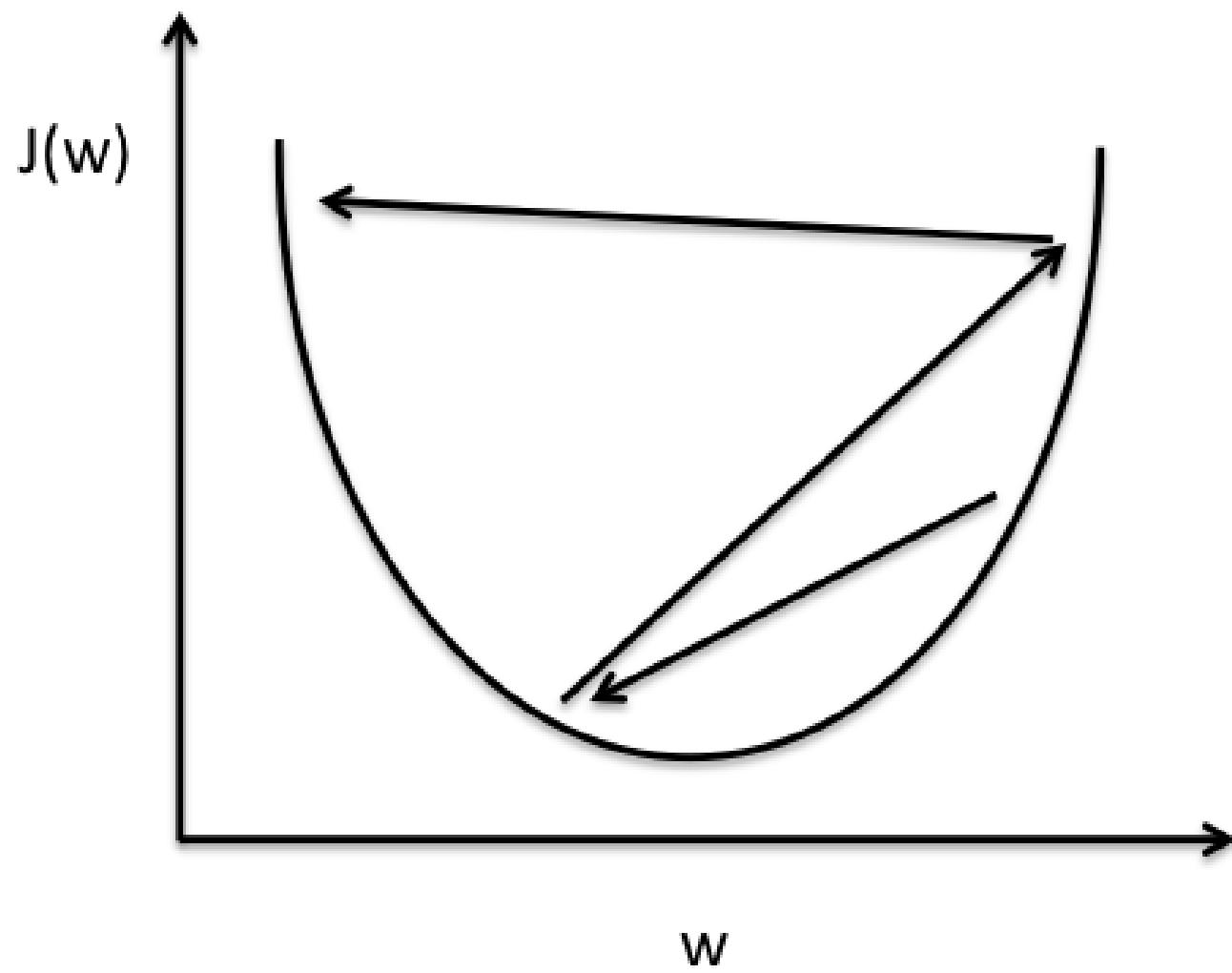
$g$  is a subgradient of  $f$  (not necessarily convex) at  $x$  if

$$f(y) \geq f(x) + \cancel{g}^T(y - x), \quad \forall y$$

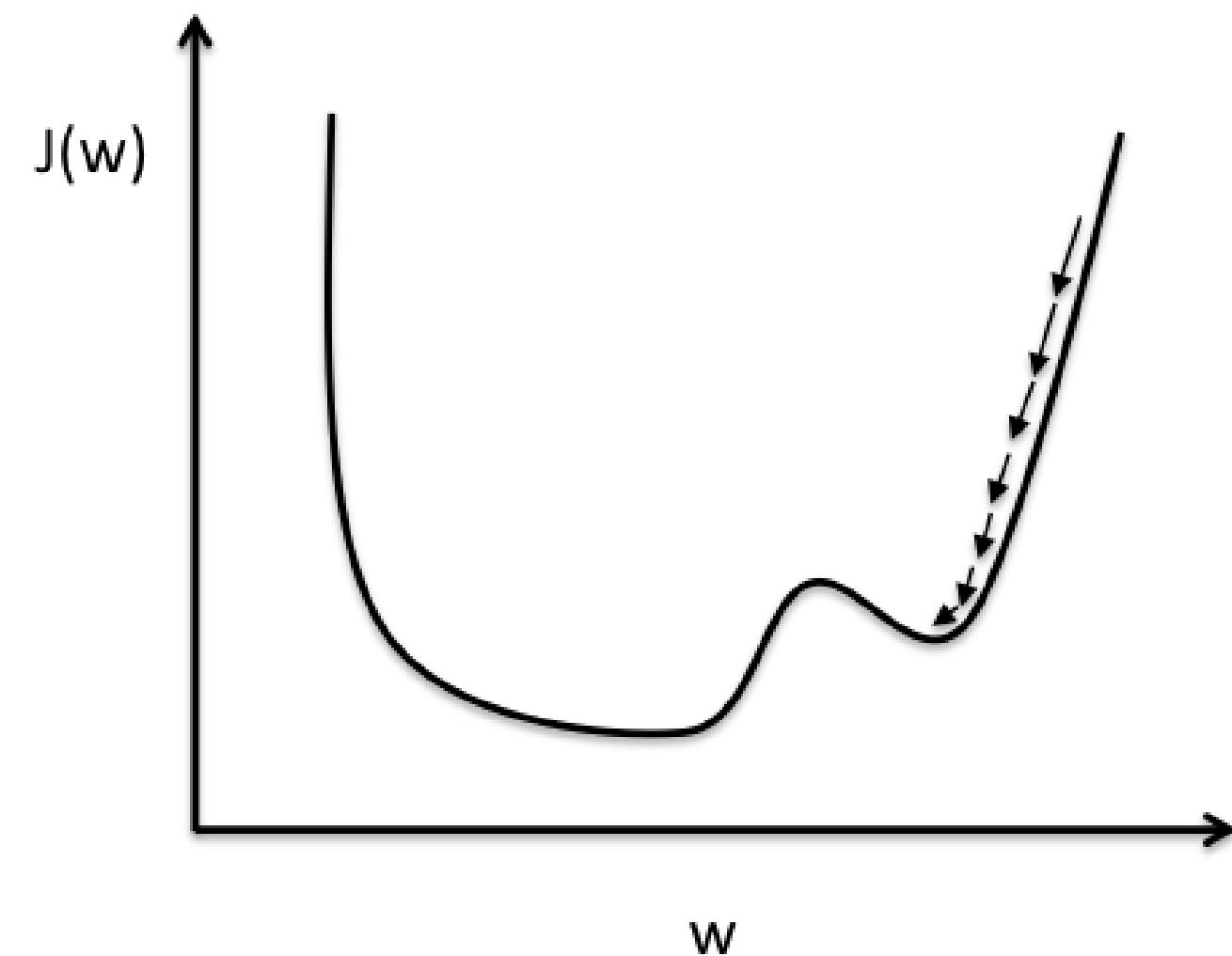


$g_2, g_3$  are subgradients at  $x_2$ ;  $g_1$  is a subgradient at  $x_1$

## Choice of step-size



Large learning rate: Overshooting.



Small learning rate: Many iterations until convergence and trapping in local minima.

## Step size rules

- ▶ Step sizes are fixed ahead of time ← [data adaptive stepsize, Adam Polyak]
- ▶ Constant step size:  $t_k = t$  (constant) 0.1, 0.2
- ▶ Constant step length:  $t_k = \gamma / \|\nabla f(x^{(k)})\|_2$  (so  $\|x^{(k+1)} - x^{(k)}\|_2 = \gamma$ )
- ▶ Square summable but not summable: step sizes satisfy

$$\sum_{k=1}^{\infty} t_k^2 < \infty, \quad \sum_{k=1}^{\infty} t_k = \infty$$

Recall page 15.

e.g.,  $t_k = 1/k$

- ▶ Nonsummable diminishing: step sizes satisfy

$$\lim_{k \rightarrow \infty} t_k = 0, \quad \sum_{k=1}^{\infty} t_k = \infty.$$

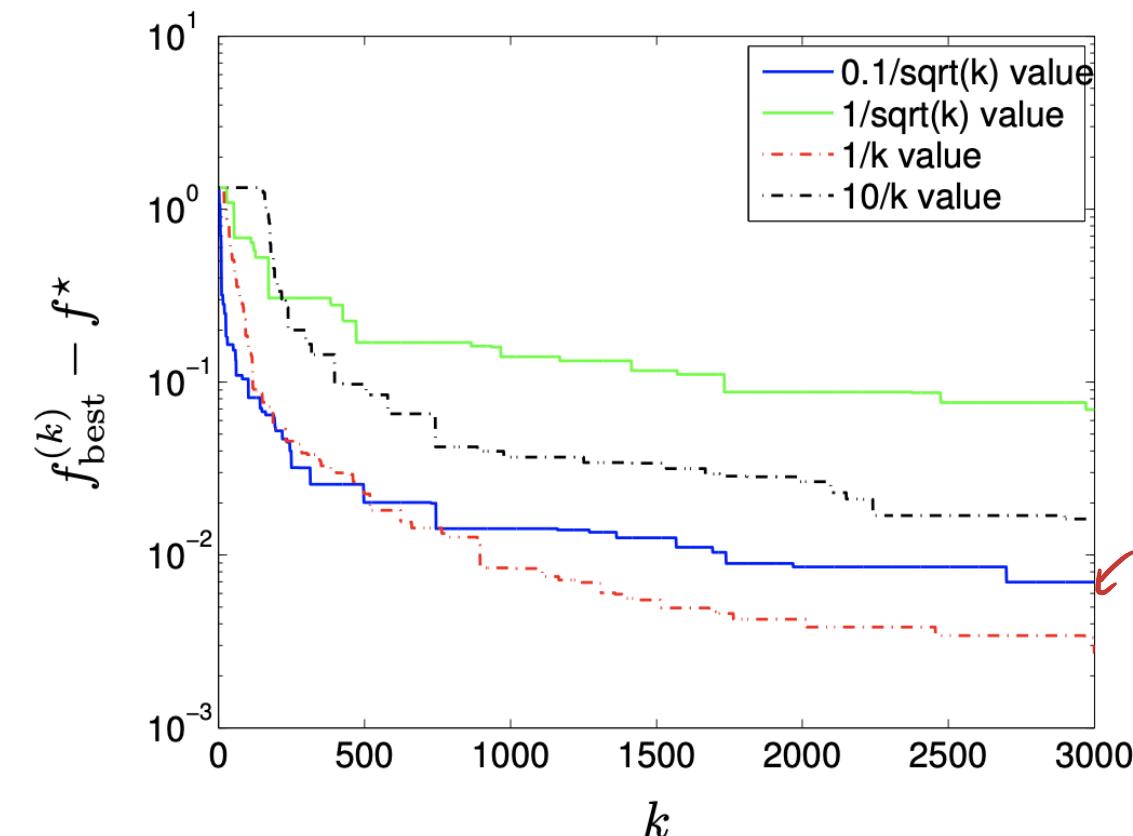
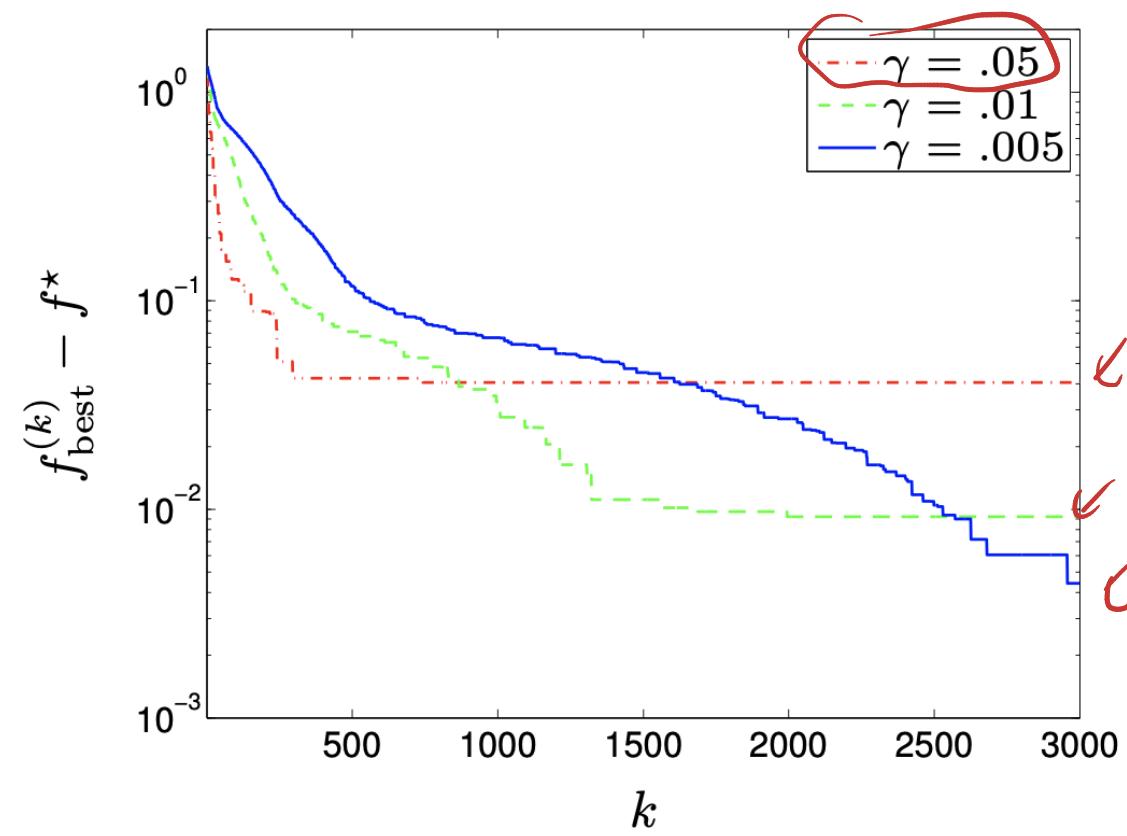
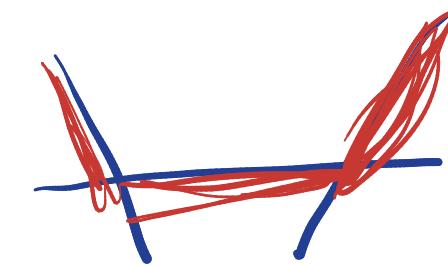
## Example

Minimizing piecewise linear function

$$\text{minimize}_{a,b} \max_{i=1,\dots,m} (a_i^T x + b_i)$$

convex

Problem instance with 20 variables.

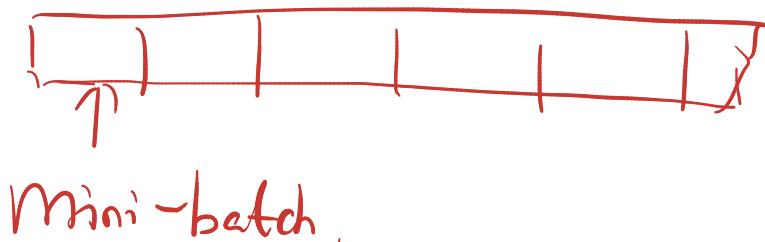


# Contents

- Gradient Descent, Stochastic Gradient Descent, Newton's Method
- **Stochastic Gradient Descent**
- Newton's Method
- Example: Solving maximum likelihood estimator for CT imaging

## Stochastic gradient descent (SGD)

$O(nP)$ .

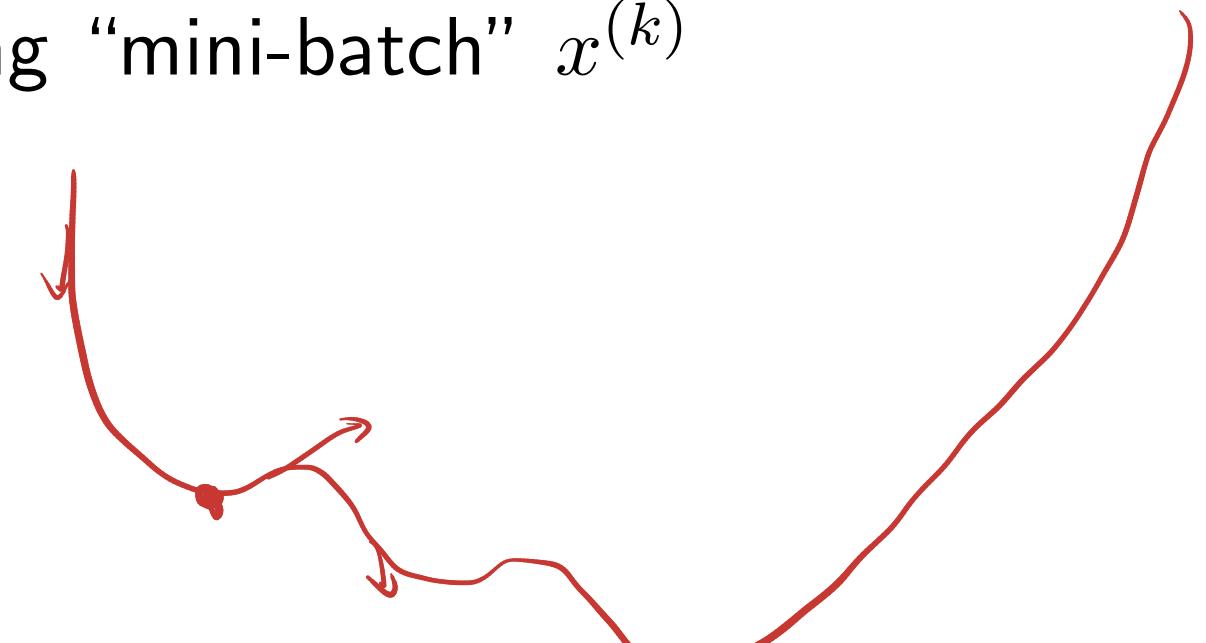


- ▶ Sequentially “load” part of data; use gradient using “mini-batches” of data
- ▶ Save memory; sometimes has better performance for non-convex problems
- ▶ Uses noisy unbiased subgradients

$$x^{(k+1)} = x^{(k)} - t_k \tilde{g}^{(k)}$$

- ▶  $\tilde{g}^{(k)}$  is any noisy unbiased estimate of gradient using “mini-batch”  $x^{(k)}$

$$\mathbb{E}[\tilde{g}^{(k)}] = g^{(k)}$$



## Stochastic gradient descent for linear regression

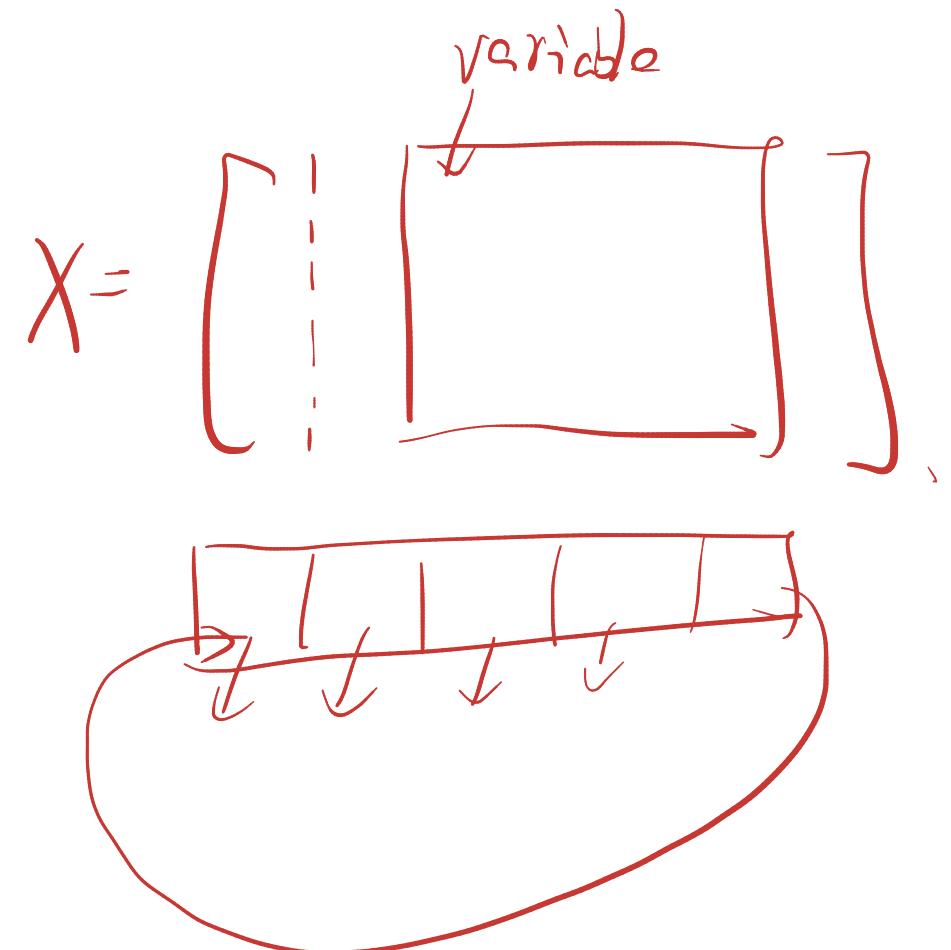
Loss function

$$\min_{\beta} \|y - X\beta\|_2^2$$

Gradient:  $f(\beta) = 2X^T(X\beta - y)$

Partition the **data** into  $M$  parts

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}, X = \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \end{bmatrix}$$



Stochastic gradient descent:

$$\beta^{(k+1)} = \beta^{(k)} - t_k \underbrace{X_k^T (X_k \beta^{(k)} - y_k)}_{\text{---}}$$

$\mathcal{O}\left(\frac{n}{M} p\right)$

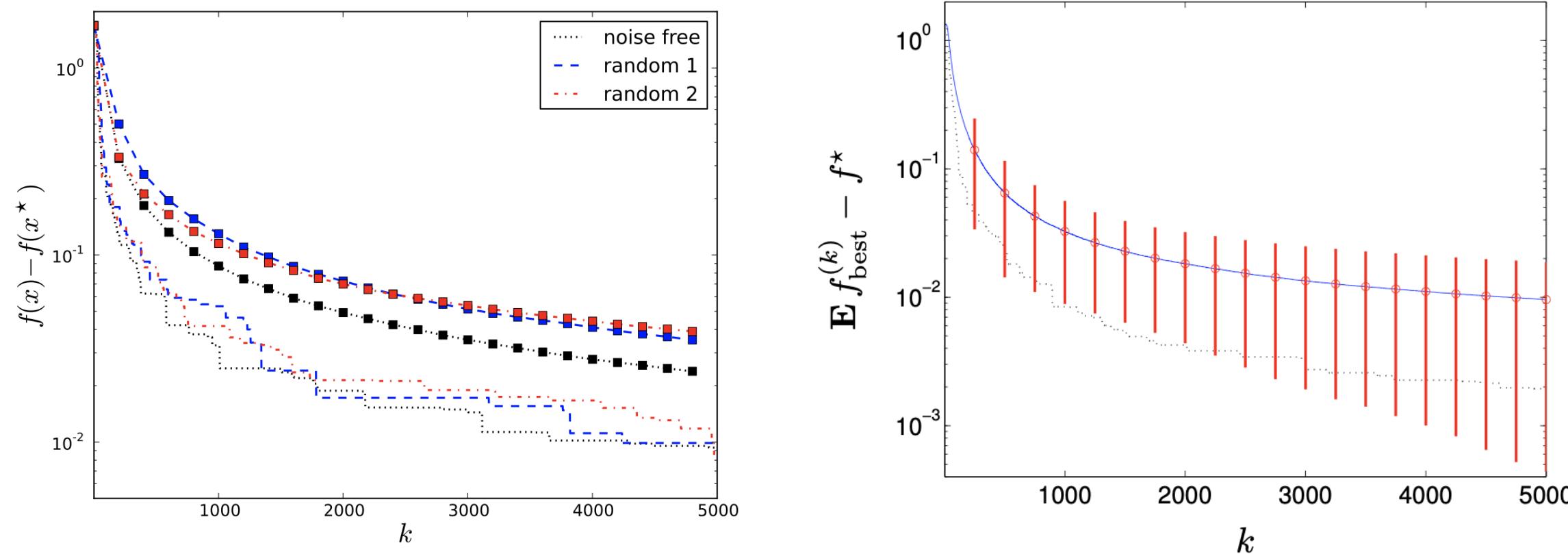
Compare with Gradient descent

$$\beta^{(k+1)} = \beta^{(k)} - t_k X^\top (X \beta^{(k)} - y)$$

$\mathcal{O}(np)$

## Example

Minimizing piecewise linear function with SGD (solid lines are averaged over 100 instances)



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## Second-order Method: Newton's method

$$x^{(k+1)} = x^{(k)} - t_k [H\{f(x^{(k)})\}]^{-1} \nabla f(x^{(k)})$$

$t_k$ : step-size for the  $k$ th iteration

- interpretation  $x + v$  minimizes the second order approximation of the function

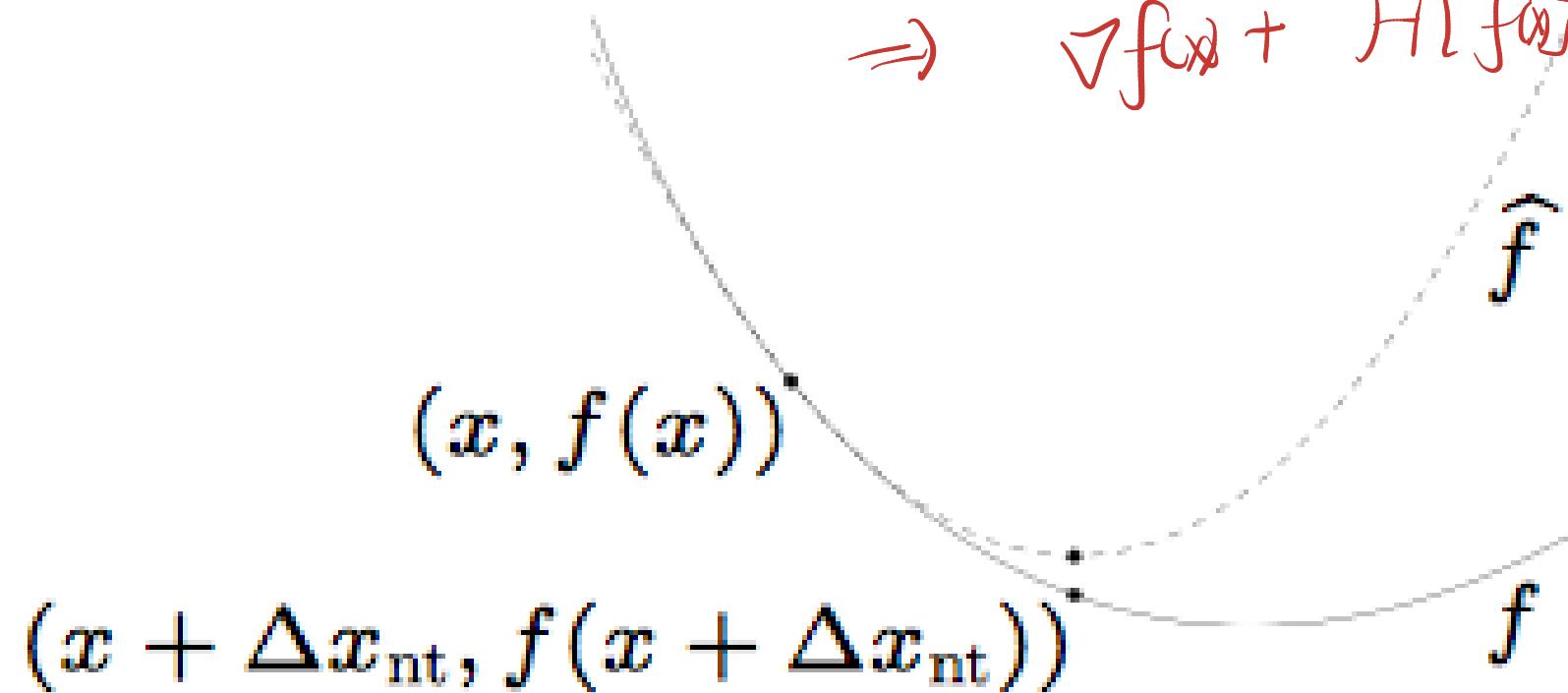
$$f(x + v) \approx f(x) + \nabla f(x)^T v + \frac{1}{2} v^T H\{f(x)\} v$$

quadratic approximation

Find  $v$  to minimize

$$\Rightarrow \nabla f(x) + H\{f(x)\}v = 0$$

$$v = -H^T\{f(x)\} \nabla f(x)$$

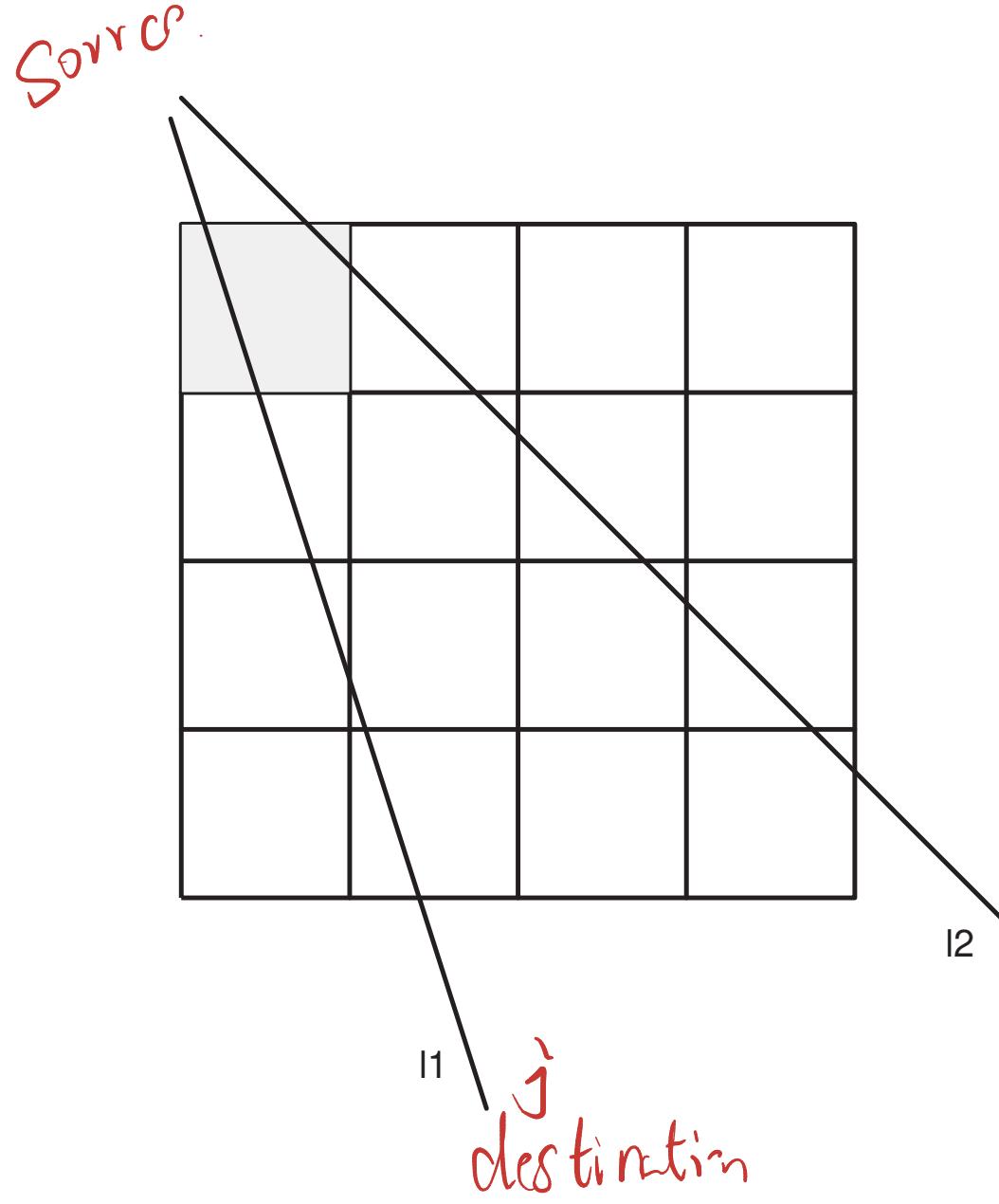


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# CT image reconstruction using MLE





- ▶  $n$  line integral measurements.
- ▶ image of size  $p \times p$
- ▶  $j$ th line is characterized by  $\{l_{ij}\}$ , where  $l_{ij}$  is the length of the intersection of  $j$ th line with  $i$ th pixel (or zero if they don't intersect)

- ▶ Measurements forms a vector  $y \in \mathbb{R}^n$

*low dose CT*

$$y_j \sim \text{Poisson}(\lambda_j), \quad j = 1, \dots, n.$$

- ▶ The parameters  $\{\lambda_j\}$  are determined according to Beer's law:

$$\lambda_j = I_j e^{-\sum_{i=1}^{p^2} l_{ij} x_j},$$

where  $I_j$  is the intensity of the  $i$ th X-ray before passing through the object.

- ▶ The problem is to reconstruct the pixel densities  $x \in \mathbb{R}^{p^2}$  from the line integral measurements  $y$ .

## Maximum likelihood estimate

- ▶ The likelihood function is given by

$$p_x(\underline{y}) = \prod_{j=1}^n \frac{\lambda_j^{y_j}}{y_j!} e^{-\lambda_j},$$

- ▶ Log-likelihood function

$$\ell(x) = \log p_x(y) = \sum_{j=1}^n (y_j \log \lambda_j - \lambda_j - \log(y_j!)).$$

- ▶ MLE estimate

$$\text{minimize}_x \quad - \sum_{j=1}^n (y_j \log \lambda_j - \lambda_j)$$

- To prevent overfitting the noisy data, we also add a regularization term  $\phi(x)$  in the cost function.

$$\underset{x}{\text{minimize}} \quad - \sum_{j=1}^n (y_j \log \lambda_j + \lambda_j) + \underbrace{\lambda \phi(x)}_{\text{Lasso.}}$$

e.g.  $\phi(x) = \|x\|_2^2$ ,  $\phi(x) = \|x\|_1$ .

- Matrix-vector representation

$$\underset{x}{\text{minimize}} \quad f(x) = y^T L x + I^T e^{-Lx} + \lambda \phi(x).$$

Forward projection matrix  $L = [l_1, \dots, l_n] \in \mathbb{R}^{n \times p^2}$ .

$I = [I_1, \dots, I_n]^T \in \mathbb{R}^n$ .

Functions  $e^x$  are overloaded to operate on each element of the input vector.

- ▶ Since  $f(x)$  is differentiable and convex, a necessary and sufficient condition for a solution  $x^*$  to be optimal is

$$\nabla f(x^*) = L^T \left( y - \text{diag}\{I\}e^{-Lx^*} \right) + \lambda \nabla \phi(x^*) = 0.$$

- ▶ Hessian matrix

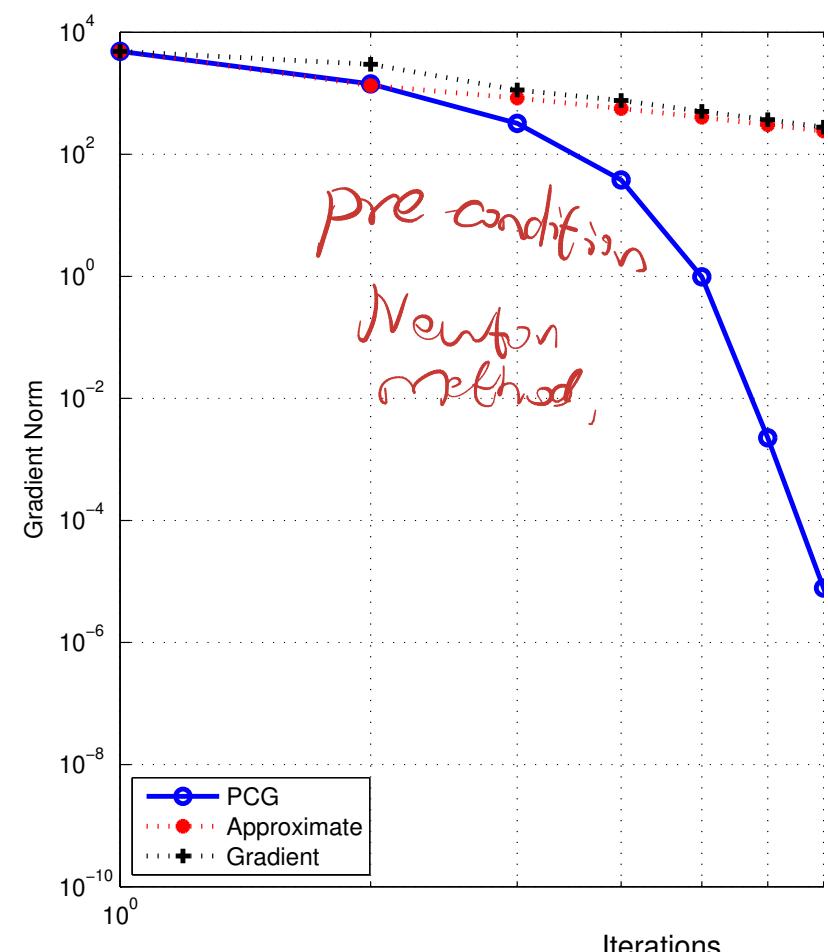
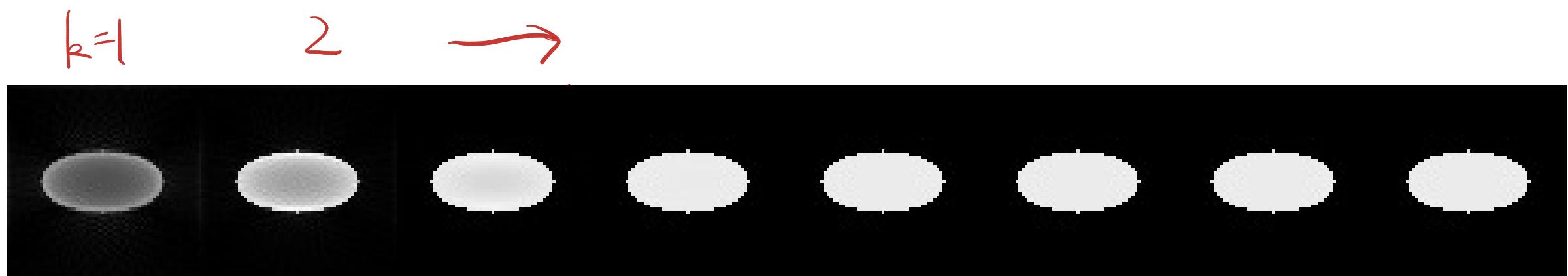
$$H = L^T \text{diag}\{\hat{y}\}L + \lambda H[\phi(x)] > 0,$$

where

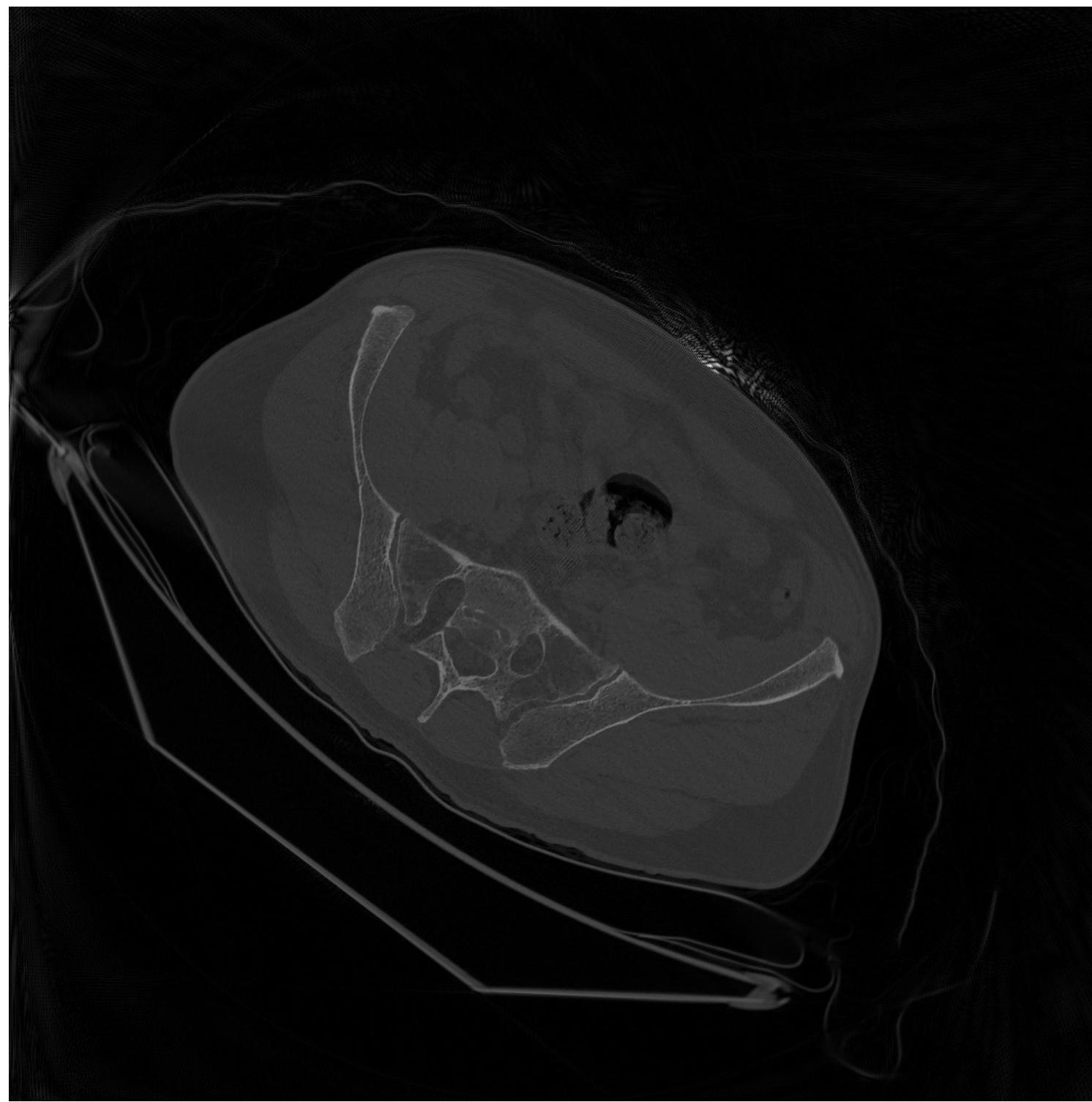
$$\hat{y} = \text{diag}\{I\}e^{-Lx}$$

## Results

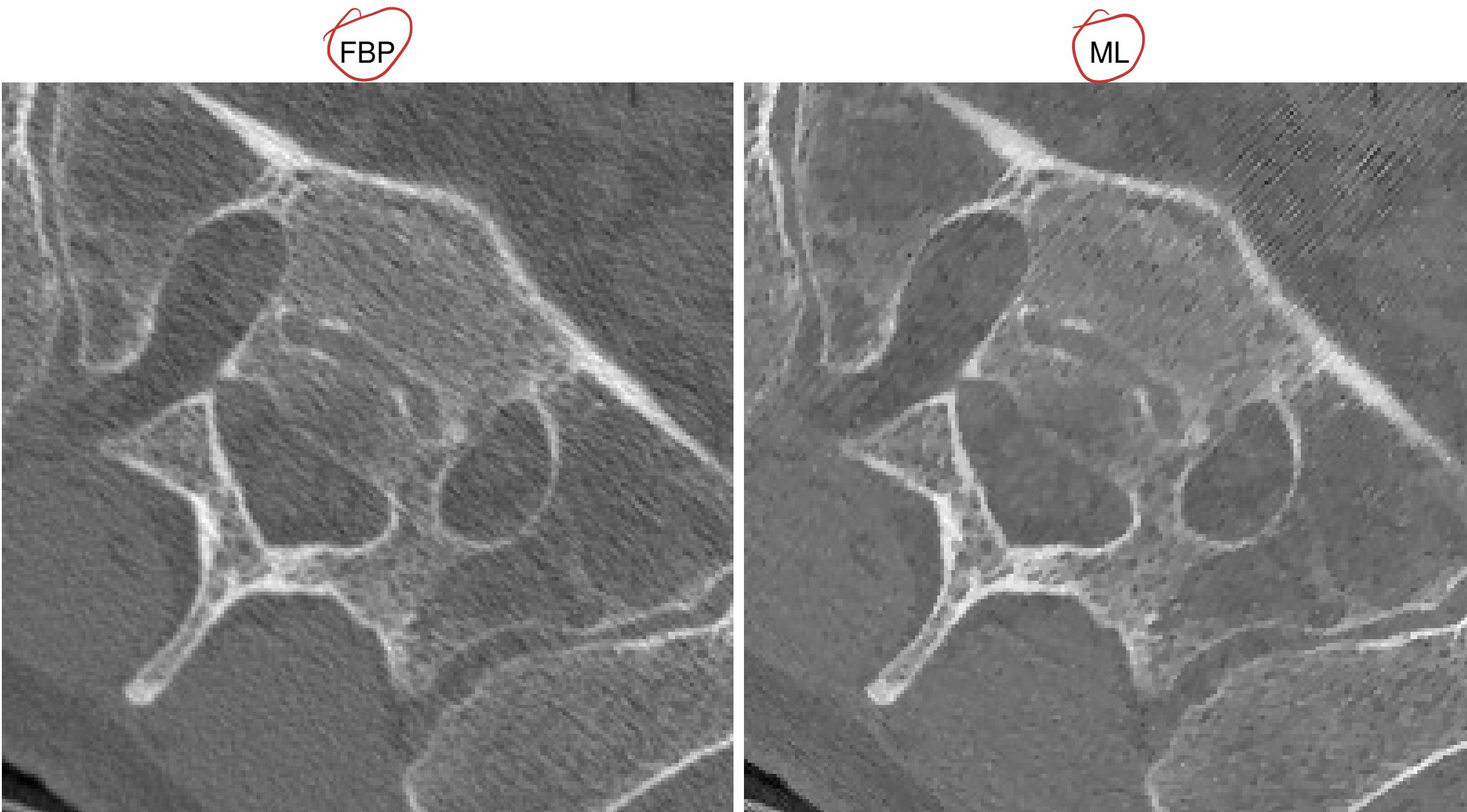
We simulated a parallel beam CT geometry, with 100 detectors, and 180 uniform angular sampling, so  $m = 18000$ . The rays spread out wide enough to cover the entire image, with uniform intensities  $I_j = 10^6$ . The image has  $64 \times 64 (= 4096)$  pixels.  
Use  $\|\nabla f\|_2 < 10^{-8}$  as a stopping criterion.



Using real data measured on a GE fan beam geometry CT scanner:  $1024 \times 1024$ .



## Comparison with a deterministic inverse algorithm



# Summary

- ▶ Gradient descent and convergence
  - ▶ Example: solving multiple linear regression, logistic regression, neural networks
  - ▶ Subgradient
  - ▶ Step-size
  - ▶ Stochastic gradient descent
- ▶ Newton's method