Optimization for Machine Learning

Nick Henderson, AJ Friend (Stanford University)
Kevin Carlberg (Meta)

August 8, 2022

Model fitting

Outline

Notation

The notation between these worlds is not consistent

- Optimization
  - f: optimization objective function
  - x: optimization variables
- Machine learning (this set of slides)
  - ϕ: optimization objective function (i.e., loss function)
  - β or θ: optimization variables (i.e., model parameters)
  - f: regression function mapping inputs to outputs
  - x: model inputs (i.e., independent variable)
  - y: model outputs (i.e., response variable)

Least-squares regression

- A type of model fitting with many applications
- **Goal**: find a model that best fits training data in the least-squares sense
- Illuminates the connection between **unconstrained optimization** and **statistics/machine learning**
- We will use the following iPython notebooks
  - `least-squares.ipynb`
  - `polynomial-fit.ipynb`
  - `smooth.ipynb`
  - `huber.ipynb`

Linear least squares: 1D case with linear data

Outline

Problem set up

- **Given**: m training examples (i.e., training set)

x_i: independent variable	y_i: response variable
0.0	0.46
0.11	0.31
0.22	0.38
0.33	0.39
0.44	0.65
0.56	0.40
0.67	0.87
0.78	0.69
0.89	0.87
1.0	0.88

- **Goal**: construct a regression model that can predict y from x

Where might these data come from?

x: independent variable	y: response variable
height	weight
square feet	price of home
device property	failure rate
stock market return	individual asset return

- Regression can be applied regardless of the origin of the data!

Regression: Approach (frequentist view)

***Goal**: construct a model that can predict y from x*

- In general, we *do not* know the mathematical model characterizing the underlying process that actually generated the data
- So, we *assume* that the data were generated from a model comprising the sum of a (deterministic) function and (stochastic) iid Gaussian noise:

$$y_i = f_{\text{true}}(x_i) + \sigma \cdot \epsilon_i, \quad i = 1, \ldots, m$$

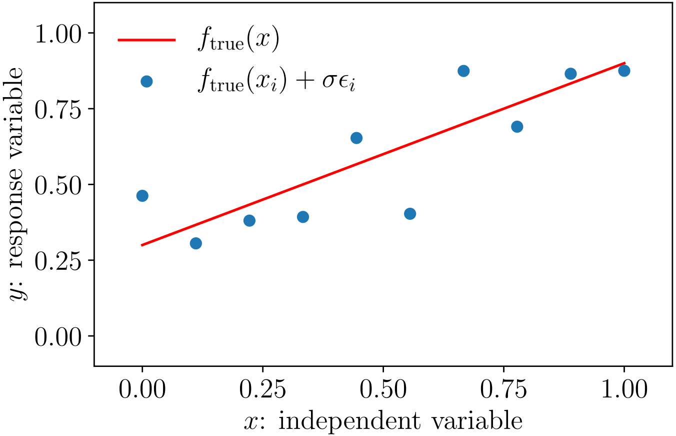
  with $f_{\text{true}}(x_i)$ unknown and $\epsilon_i \sim N(0,1)$
- We aim to construct $f(x)$ such that $f(x) \approx f_{\text{true}}(x)$ in some sense
- This is known as *regression* and is performed via optimization
  - *objective function*: residual sum of squares $\frac{1}{2}\sum_{i=1}^{m}(f(x_i) - y_i)^2$
  - *optimization variables*: parameters within the assumed form of $f(x)$
- Then, we can make predictions $y \approx f(x)$ for new values of x.

Follow along in Python

- See `least-squares.ipynb`
- In this case, we have set $f_{\text{true}}(x) = \theta_{\text{true}} \cdot x_i + b_{\text{true}}$ and $\sigma = 0.1$
  - $\theta_{\text{true}} = 0.6$
  - $b_{\text{true}} = 0.3$
- Run the first three cells of `least-squares.ipynb`
- Python code to generate data (in second cell):

```
np.random.seed(1)
theta = 0.6
b = 0.3
sigma = .1
x = np.linspace(0,1,10)
y = theta*x + b + sigma*np.random.standard_normal(x.shape)
```

Plot the data



The residuals

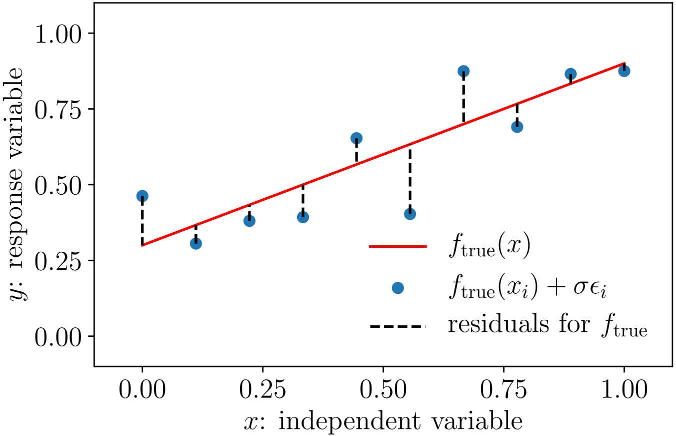
- Any given data point will result in some error or **residual**

$$r_i = f(x_i) - y_i$$

- Due to the Gaussian noise, $y_i = f_{\text{true}}(x_i) + \sigma \cdot \epsilon_i \neq f_{\text{true}}(x_i)$. Thus, the true function $f_{\text{true}}(x)$ will yield residuals

$$r_{\mathsf{true},i} = f_{\mathsf{true}}(x_i) - y_i = -\sigma \cdot \epsilon_i$$

The residuals for $f_{\text{true}}(x)$



Linear regression in one dimension

- In linear regression, we enforce the regression function $f(x)$ to be linear

$$f(x; \theta, b) = \theta \cdot x + b$$

  - regression function has two parameters: the slope θ and the y-intercept b
  - semicolon separates model input from model parameters
- **Note**: the form of $f(x)$ usually does not match the (generally unknown) form of $f_{\text{true}}(x)$. We are lucky if this happens!

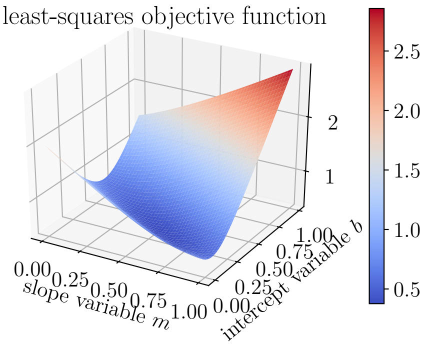
Fit the model via optimization

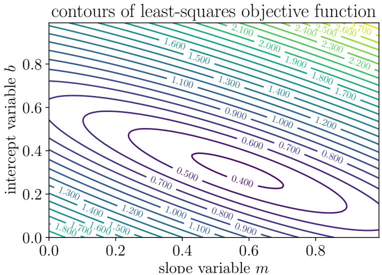
- Given training data $(x_i, y_i)_{i=1}^m$ with $x_i \in \mathbf{R}$ and $y_i \in \mathbf{R}$
- To fit the model, construct an optimization problem

$$\underset{\theta,b}{\text{minimize}} \quad \phi(\theta, b) = \frac{1}{2}\sum_{i=1}^m r_i(\theta, b)^2 = \frac{1}{2}\sum_{i=1}^m (f(x_i; \theta, b) - y_i)^2$$

  - *Optimization objective function*: residual sum of squares (RSS)
    - one contribution from each of the m training examples
  - *Optimization variables*: parameters θ and b
- Assuming the true underlying model actually is $y_i = \theta_{\text{true}} \cdot x_i + b_{\text{true}} + \sigma \cdot \epsilon_i$ with ϵ_i mean-zero Gaussian, then θ and b are the maximum-likelihood estimates of θ_{true} and b_{true}

Objective function





- The objective function $\phi(\theta, b)$ is appears to be convex (it is!)
- The global minimum occurs around $\theta^{\star} \approx 0.6$ and $b^{\star} \approx 0.35$

Optimizing by hand

Recall the sufficient conditions for (unconstrained) optimality:

1. $\nabla\phi(\theta^\star, b^\star) = 0$
2. $\nabla^2\phi(\theta^\star, b^\star) \succ 0$. **This holds everywhere!**
   - The objective function is strongly convex
   - This simplifies things: we only need to find a stationary point satisfying condition 1
   - This is one reason why convex optimization is so nice!

Let's compute $\theta^\star$ and $b^\star$ such that that the first condition holds.

Compute gradient analytically and set to zero

Analytical gradient computation:

$$\frac{\partial \phi}{\partial \theta} = \frac{1}{2} \sum_{i=1}^{m} \frac{\partial}{\partial \theta} (\theta \cdot x_i + b - y_i)^2 = \theta \sum x_i^2 + b \sum x_i - \sum x_i y_i$$

$$\frac{\partial \phi}{\partial b} = \frac{1}{2} \sum_{i=1}^{m} \frac{\partial}{\partial b} (\theta \cdot x_i + b - y_i)^2 = \theta \sum x_i + nb - \sum y_i$$

Set analytical gradient to zero and obtain a system of equations:

$$\frac{\partial \phi}{\partial \theta} = 0$$

$$\frac{\partial \phi}{\partial b} = 0$$

Solution

$$\theta = \frac{\sum x_i y_i - \frac{1}{m}\sum x_i \sum y_i}{\sum x_i^2 - \frac{1}{m}(\sum x_i)^2}$$

$$b = \frac{\sum y_i - \theta \sum x_i}{m}$$

Let's look at θ

Something looks nice here:

$$\theta = \frac{\sum x_i y_i - \frac{1}{m}\sum x_i \sum y_i}{\sum x_i^2 - \frac{1}{m}(\sum x_i)^2}$$

Multiply both numerator and denominator by $1/m$:

$$\theta = \frac{\frac{1}{m}\sum x_i y_i - \frac{1}{m}\sum x_i \frac{1}{m}\sum y_i}{\frac{1}{m}\sum x_i^2 - (\frac{1}{m}\sum x_i)^2}$$

We see sample covariance and variance here!

$$\theta = \frac{\mathsf{cov}(X, Y)}{\mathsf{var}(X)}$$

Let's solve in Python!

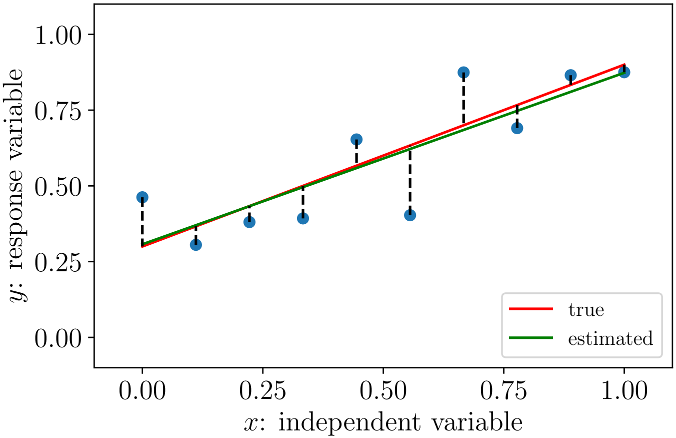
Code:

```
# solve via numpy covariance function
A = np.vstack((x,y))
V = np.cov(A)
theta_est = V[0,1] / V[0,0]
b_est = (y.sum() - theta_est*x.sum()) / len(x)
print(theta_est)
print(b_est)
```

Result:

```
theta_est = 0.56604 (true value = 0.6)
b_est = 0.30727 (true value = 0.3)
```

Look at the plot



Solve in CVXPY

Remember the optimization problem: minimize $\frac{1}{2}\sum_{i=1}^{m}(\theta \cdot x_i + b - y_i)^2$

We can write this directly in CVXPY:

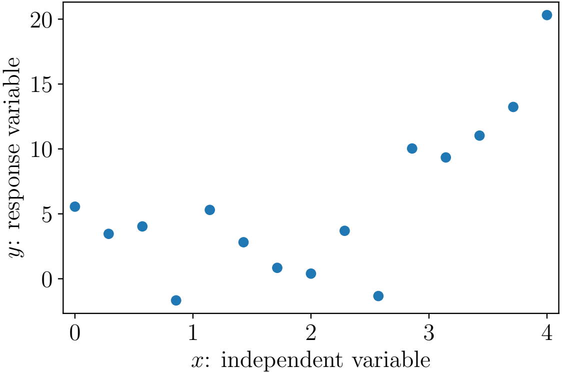
```
from cvxpy import *
# Construct the problem.
theta_cvx = Variable()
b_cvx = Variable()
objective = Minimize(sum_squares(theta_cvx*x + b_cvx - y))
prob = Problem(objective)
# The optimal objective is returned by prob.solve().
result = prob.solve()
```

```
theta_cvx.value = 0.56604, b_cvx.value = 0.30727
```

Linear least squares: 1D case with non-linear data

Outline

What about these data?

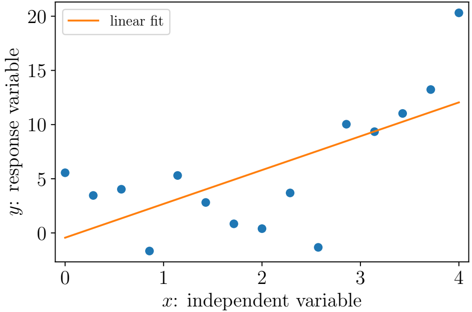


- Here, $f_{\text{true}}(x) = \theta_{\text{true}} \exp(x) + b_{\text{true}}$, which we do not know
- We just have access to the data!

We could fit a linear model

- Given our ignorance of f_{true}, we could fit a linear model

$$f(x;\theta,b) = \theta \cdot x + b,$$



- This yields an objective-function value of $\phi(\theta, b) = 283.63$

We can also fit an exponential model

- If we think that the underlying model may be exponential, we can also try

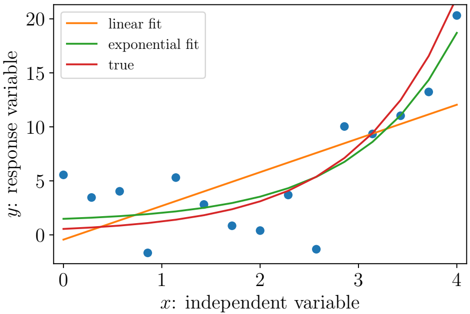
$$f(x; \theta, b) = \theta \cdot \exp(x) + b$$

  - Model still **linear in the parameters** θ **and** b: "Linear least squares" (same optimization problem)
  - But model **nonlinear in the independent variable** x: "Nonlinear regression"

CVXPY code:

```
theta = Variable()
b = Variable()
objective = Minimize(sum_squares(theta*np.exp(x) + b - y))
prob = Problem(objective)
result = prob.solve()
```

Result



- This yields a *smaller* objective-function value of $\phi(\theta, b) = 122.80$
  - better fit to training data
- **Caution**: can overfit training data
  - must assess generalization error on an independent test set

Linear least squares: general formulation and matrix–vector form

Outline

General formulation for linear least squares

- $x \in \mathbf{R}^p$: p-dimensional model inputs (i.e., independent variables)
- $y \in \mathbf{R}$: model outputs (i.e., response variable)
- $f : \mathbf{R}^p \to \mathbf{R}$: model a **linear combination** of n functions $f_i : \mathbf{R}^n \to \mathbf{R}$, $i = 1, \ldots, n$:

$$f(x; \beta) = \sum_{i=1}^{n} f_i(x)\beta_i$$

  - If f_i is nonlinear in x, then this is "nonlinear regression"
  - *Previous example*: $n = 2$; $f_1(x) = 1$; $f_2(x) = x$ or $f_2(x) = \exp(x)$; $\beta_1 = \theta$, $\beta_2 = b$
- $\beta = (\beta_1, \ldots, \beta_n) \in \mathbf{R}^n$: optimization variables (i.e., model parameters)

Matrix–vector form

- Assume input–output data of the form $(x_j, y_j)_{j=1}^m$
- The residual for the jth data point is $r_j(\beta) = f(x_j; \beta) - y_j$
- Residual sum of squares (RSS) objective function is

$$\phi(\beta) = \frac{1}{2}\sum_{j=1}^{m} r_j(\beta)^2 = \frac{1}{2}\sum_{j=1}^{m}(f(x_j;\beta) - y_j)^2 = \frac{1}{2}\sum_{j=1}^{m}(\sum_{i=1}^{n} f_i(x_j)\beta_i - y_j)^2$$

- Defining

$$A = \begin{bmatrix} f_1(x_1) & \cdots & f_n(x_1) \\ \vdots & \ddots & \vdots \\ f_1(x_m) & \cdots & f_n(x_m) \end{bmatrix}, \qquad \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_n \end{bmatrix}, \qquad b = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

we can write the objective function as $\boxed{\phi(\beta) = \frac{1}{2}\|A\beta - b\|_2^2}$

Standard form for least squares

$$\underset{x}{\text{minimize}} \quad \tfrac{1}{2}||Ax - b||_2^2$$

In the context of model fitting:

- $A \in \mathbf{R}^{m\times n}$ is the matrix that contains data from independent variables
- $b \in \mathbf{R}^{m}$ is the vector containing response data (β on last slide)
- $x \in \mathbf{R}^{n}$ is the vector of model parameters
- For each of the m training examples, the residual is we have the equation

$$r_i = a_i^T x - b_i,$$

  - $a_i^T \in \mathbf{R}^{1\times n}$ is the ith row of A
- Notation from statistics:

$$\underset{\beta}{\text{minimize}} \frac{1}{2}||\mathbf{X}\beta - \mathbf{y}||_2^2$$

CVXPY for least squares

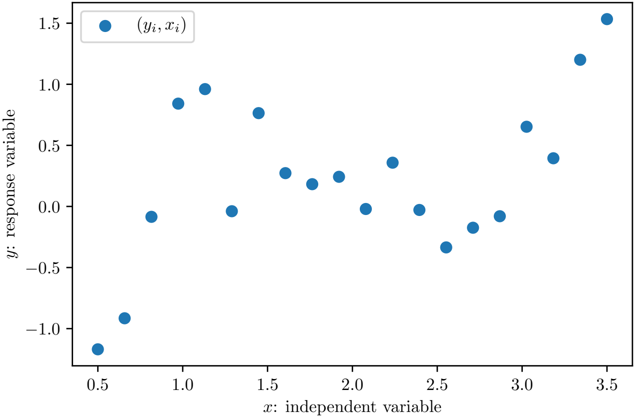
```
# generate input and response data
np.random.seed(1); n = 10 # number of data points
input_data = np.linspace(0,1,n)
response_data = 0.6*input_data + 0.3 + 0.1*np.random.standard_normal(n)
# least-squares matrix and vector
A = np.vstack([input_data,np.ones(n)]).T; b = response_data
# CVX problem
x = Variable(A.shape[1])
objective = Minimize(sum_squares(A*x - b))
prob = Problem(objective); result = prob.solve()
# get value & print
x_star = np.array(x.value)
print('slope = {:.4}, intercept = {:.4}'.format(x_star[0,0],x_star[1,0]))
```

```
slope = 0.566, intercept = 0.3073
```

Examples

Outline

What about these data?



Polynomial regression

- Polynomial model:

$$y \approx f(x;\beta) = \beta_1 + \beta_2 x + \beta_3 x^2 + \cdots + \beta_n x^{n-1}$$

- β_i, $i = 1, \ldots, n$ are the model parameters and optimization variables
- Linear least-squares framework: $f(x) = \sum_{i=1}^{n} f_i(x)\beta_i$ with monomials

$$f_i(x) = x^{i-1},\ i = 1, \ldots, n$$

Polynomial regression

- As before, define A, β, b to put in standard form for least squares

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ 1 & x_3 & x_3^2 & \dots & x_3^{n-1} \\ 1 & x_4 & x_4^2 & \dots & x_4^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^{n-1} \end{bmatrix}, \qquad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \vdots \\ \beta_n \end{bmatrix}, \qquad b = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ \vdots \\ y_m \end{bmatrix}$$

- Solve the least-squares problem

$$\underset{\beta}{\text{minimize}} \quad \frac{1}{2}\|A\beta - b\|_2^2$$

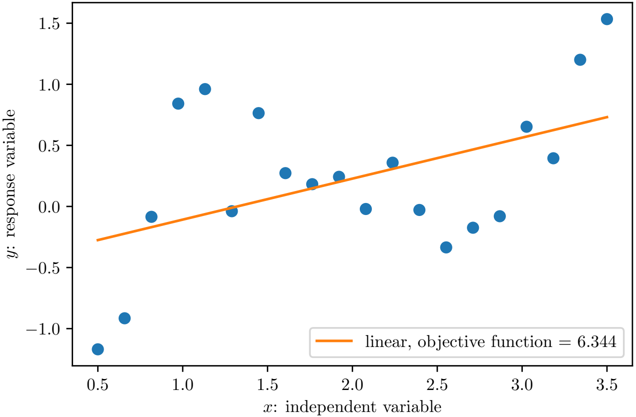
- This form for A is called the **Vandermonde matrix**

Solve with CVXPY

- See `polynomial-fit.ipynb`

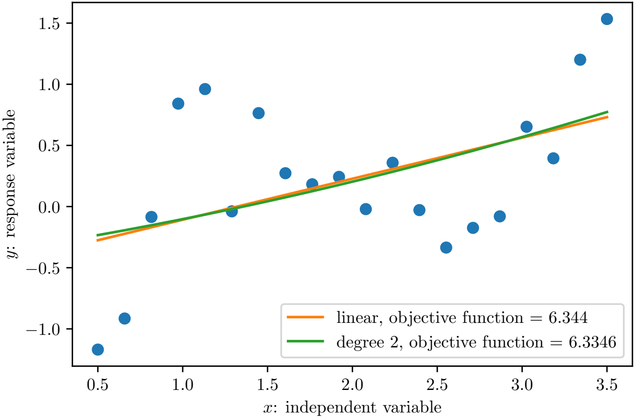
```
def cvxpy_poly_fit(x,y,degree):
    # construct data matrix
    A = np.vander(x,degree+1)
    b = y
    beta_cvx = Variable(degree+1)
    # set up optimization problem
    objective = Minimize(sum_squares(A*beta_cvx - b))
    constraints = []
    # solve the problem
    prob = Problem(objective,constraints)
    prob.solve()
    # return the polynomial coefficients
    return np.array(beta_cvx.value)
```

Linear fit

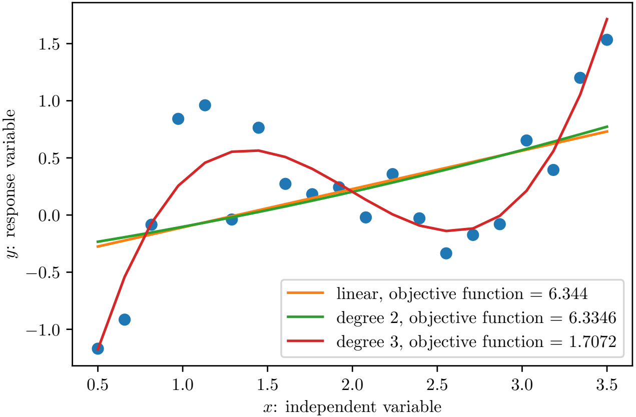


1.5
1.0
0.5
0.0
−0.5
−1.0
y: response variable
linear, objective function = 6.344
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x: independent variable

Quadratic fit

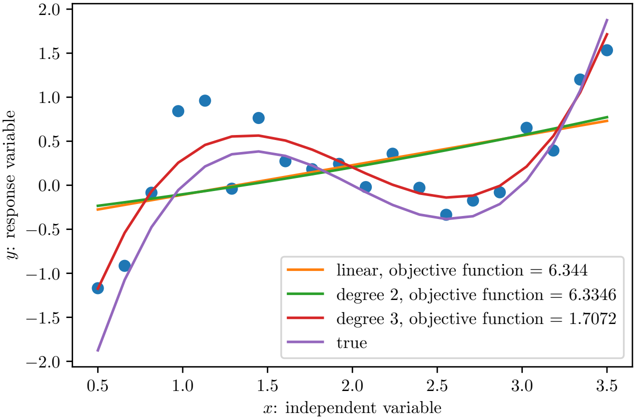


Cubic fit



1.5
1.0
0.5
0.0
−0.5
−1.0
y: response variable
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x: independent variable
linear, objective function = 6.344
degree 2, objective function = 6.3346
degree 3, objective function = 1.7072

True model

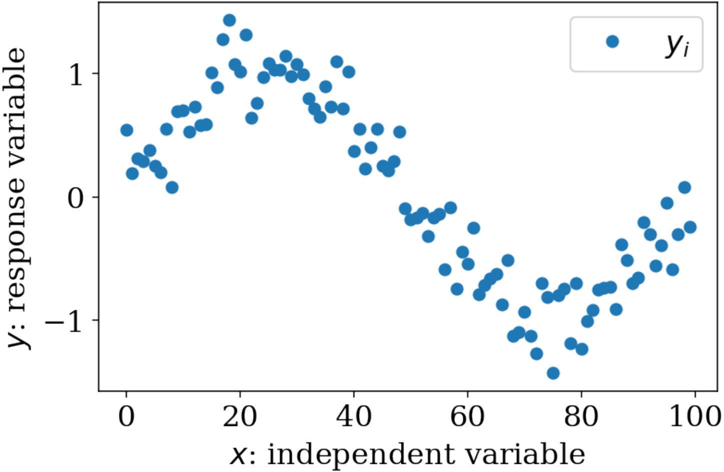


▶ This was the true (but unknown) model that generated the data

Example: time series smoothing

- See `smooth.ipynb`
- Noisy observations (x_i, y_i), $i = 1, \ldots, m$ at regular intervals (discretized curve)
- New modeling approach
  - We assume we **don't** have a model for the curve (linear, polynomial, ...)
  - But we **do** believe that the curve should be smooth
- **Idea**: find β_i, $i = 1, \ldots, m$ that are *close* to y_i, but are *penalized* for being nonsmooth
  - Linear least squares with $f_i(x_j) = \delta_{ij}(x_j)$, $i = 1, \ldots, m$ (Kronecker delta)
  - The number of optimization variables n is equal to number of data points m
  - A **non-parametric** approach

Time series data



Optimization problem: non-parametric modeling

- Want $\beta_i \approx y_i$, $i = 1, \dots, m$
- Want $f(x_j) = \sum_{i=1}^{n} \delta_{ij}(x_j)\beta_i$ to be smooth on the grid x_j, $j = 1, \dots, m$
- Optimization problem

$$\underset{\beta}{\text{minimize}} \ ||\beta - y||_2^2 + \rho \cdot \text{penalty}(\beta)$$

- Introduce a penalty function to encourage smoothness
- Penalty parameter ρ enables trading off two competing objectives:
  1. ρ small: $||\beta - y||_2^2$ small and model is a better fit to training data
  2. ρ large: penalty(β) small and model is smoother

How to quantify smoothness?

- Smoothness: a curve whose *slope does not change much*
- The second derivative measures the rate of change of the slope
- Approximate the second derivative via second-order finite differences as $D\beta$, where

$$D = \begin{pmatrix} 1 & -2 & 1 & 0 & \dots & & & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & & 0 \\ 0 & 0 & 1 & -2 & -1 & 0 & \dots & 0 \\ \vdots & & & & & & & \end{pmatrix}$$

assuming a uniform grid x_j, $j = 1, \dots, m$.

Least-squares model: non-parametric modeling

- Updated optimization problem:

$$\underset{\beta}{\text{minimize}} \quad \|\beta - y\|_2^2 + \rho\|D\beta\|_2^2$$

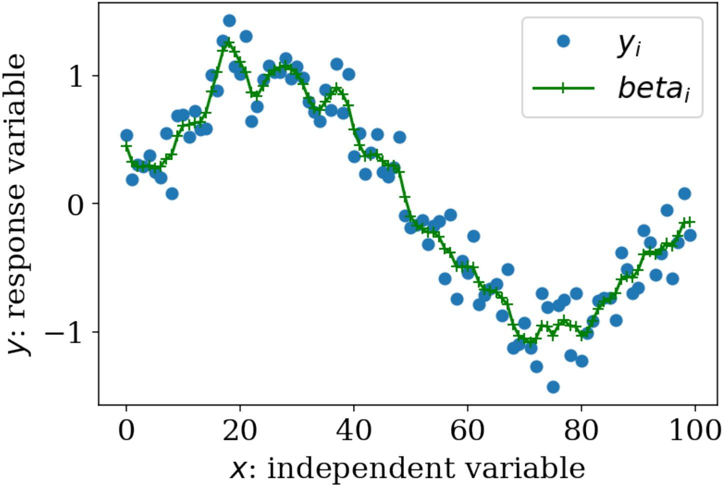
- Standard form:

$$\underset{\beta}{\text{minimize}} \left\| \begin{pmatrix} I \\ \rho D \end{pmatrix} \beta - \begin{pmatrix} y \\ 0 \end{pmatrix} \right\|_2^2$$

Solve the problem in CVXPY

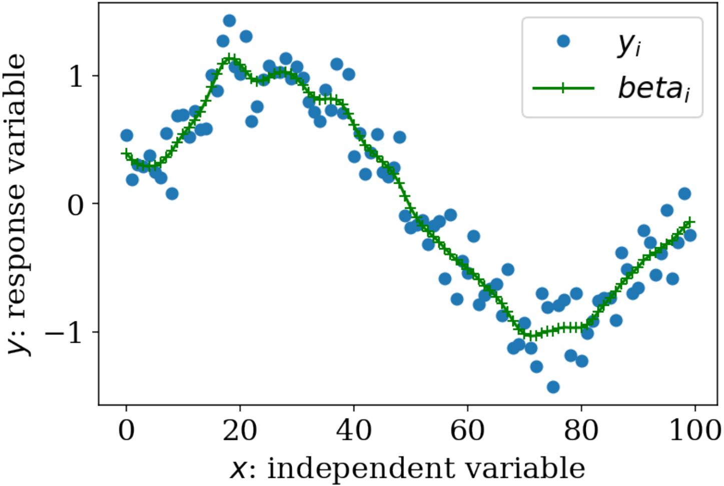
```
# get second-order difference matrix
D = diff(n, 2) # user-defined function
rho = 1
# construct and solve problem
beta = cvx.Variable(n)
cvx.Problem(cvx.Minimize(cvx.sum_squares(beta-y)
                         +rho*cvx.sum_squares(D*beta))).solve()
beta = np.array(beta.value).flatten()
```

$\rho = 1$



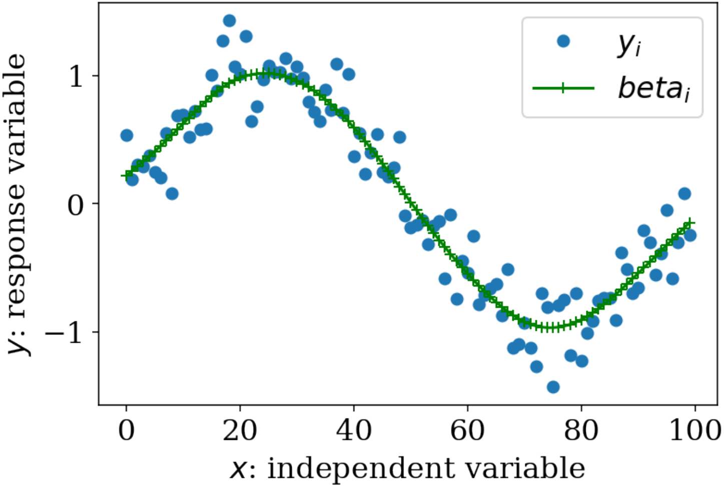
y_i
$beta_i$
1
0
−1
0
20
40
60
80
100
y: response variable
x: independent variable

$\rho = 10$



1
0
−1
0
20
40
60
80
100
y: response variable
x: independent variable
y_i
$beta_i$

$\rho = 1000$



y_i
$beta_i$
1
0
−1
y: response variable
0
20
40
60
80
100
x: independent variable

Nonlinear least squares

Outline

Nonlinear least squares

Linear least squares:

1. Model is *linear in the parameters*

$$f(x;\beta) = \sum_{i=1}^{n} \beta_i f_i(x)$$

   - *Linear regression*: f_i is also linear in x
   - *Nonlinear regression*: f_i is nonlinear in x (e.g., polynomials, exponential)
2. Minimize the residual sum of squares (RSS)

Nonlinear least squares:

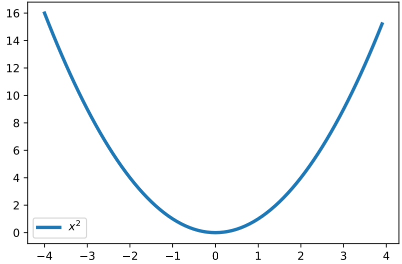
1. Model $f(x;\beta)$ is *nonlinear in the parameters* β
2. Minimize the same objective function: residual sum of squares (RSS)
   - Again equivalent to maximum likelihood if additive Gaussian noise
   - Algorithms: line-search (Gauss–Newton) and trust-region (Levenberg–Marquardt)

Beyond least squares

Outline

Quadratic loss function

- See `huber.ipynb`
- Least squares employs a quadratic loss function

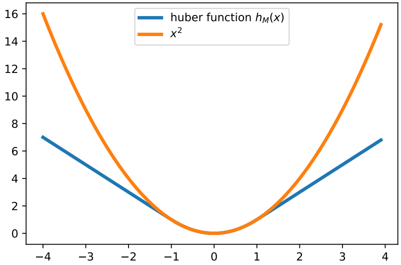


- This function imposes a severe penalty on large values
- As a result, the fit model is very sensitive to outliers
- Can we use a different loss function?

Huber loss function

- The Huber function allows us to better handle outliers in data
  - Usual quadratic loss in interval $[-M, M]$
  - Linear loss for $|x| > M$

$$h_M(x) = \begin{cases} x^2 & |x| \leq M \\ 2M|x| - M^2 & |x| > M \end{cases}$$



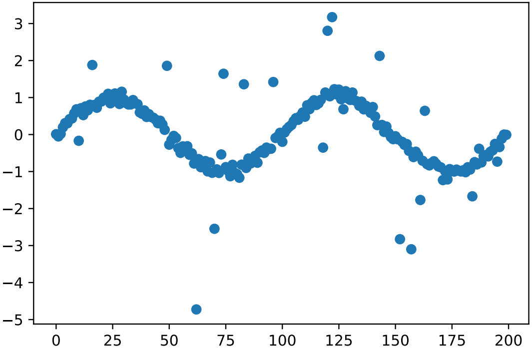
Huber loss function

- This function imposes a less severe penalty on large values
- Let's repeat the time-series example, but include extreme outliers
- Penalize closeness to data with Huber function h_M to reduce outlier influence:

$$\underset{\beta}{\text{minimize}} \quad \textstyle\sum_{i=1}^{m} h_M(\beta_i - y_i) + \rho\|D\beta\|_2^2$$

    - M parameter controls width of quadratic region, or "non-outlier" errors
- This is no longer least squares!
- CVXPY has implemented the Huber loss function

Huber data

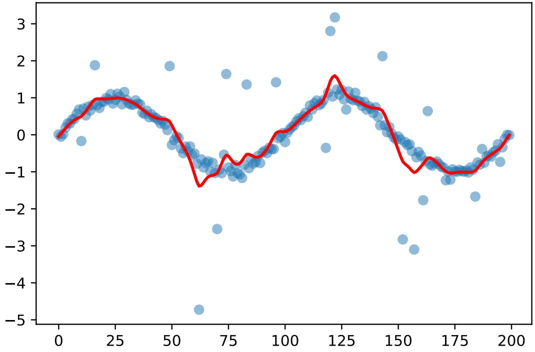


Least-squares smoothing

```
# get second-order difference matrix
D = diff(n, 2)
rho = 20

beta = Variable(n)
obj = sum_squares(beta-y) + rho*sum_squares(D*beta)
Problem(Minimize(obj)).solve()
beta = np.array(beta.value).flatten()
```

Least-squares smoothing result



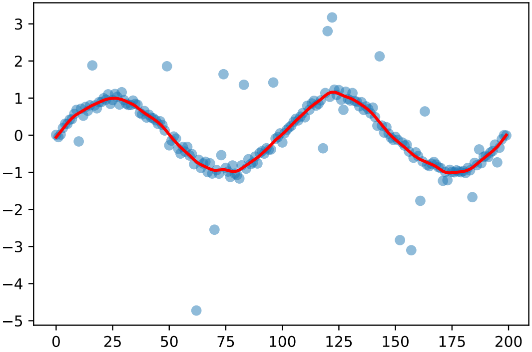
- Model overfits the outliers

Huber smoothing

```
# get second-order difference matrix
D = diff(n, 2)
rho = 20
M = .15 # huber radius

beta = Variable(n)
obj = sum_entries(huber(beta-y, M)) + rho*sum_squares(D*beta)
Problem(Minimize(obj)).solve()
x = np.array(x.value).flatten()
```

Huber smoothing result



- The model is less sensitive to outliers!

Deep Neural Networks

Outline

Deep Neural Networks

A deep neural network defineds a particular model $f(x;\beta)$

- $f(x;\beta) = f^{(3)}(f^{(2)}(f^{(1)}(x;\beta_1);\beta_2);\beta_3)$ is a 'network' (function composition)
  - $f^{(i)}(x;\beta_i)$: function charactering the ith layer with parameters β_i
  - parameters $\beta = (\beta_1, \beta_2, \beta_3) \in \mathbf{R}^n$
- Evaluating f is 'forward propagation': start at the beginning ($f^{(1)}$) and evaluate forward sequentially
- It is 'deep' if there are many (≥ 4) composed functions, and thus β is often high-dimensional
- f is generally nonlinear in the parameters β
- if additive Gaussian noise, then MLE leads to nonlinear least squares
- other loss functions possible (e.g., non-Gaussian noise); then no longer least squares

Deep Feedforward Networks

- Computing the gradient can be done by applying the chain rule, e.g.,

$$\frac{\partial \phi}{\partial \beta_2} = \frac{\partial \phi}{\partial f^{(3)}} \frac{\partial f^{(3)}}{\partial x} \frac{\partial f^{(2)}}{\partial \beta_2}, \qquad \frac{\partial \phi}{\partial \beta_1} = \frac{\partial \phi}{\partial f^{(3)}} \frac{\partial f^{(3)}}{\partial x} \frac{\partial f^{(2)}}{\partial x} \frac{\partial f^{(1)}}{\partial \beta_1}$$

- Computing the gradient from left to right is referred to as reverse-mode automatic differentiation or **back propagation**: the chain rule 'propagates' information from the end of the network ($f^{(3)}$) upstream (e.g., to $f^{(1)}$)
  - More efficient if input dimension larger than output dimension, which is true in model fitting (output dimension is one)
- Computing the gradient from left to right is referred to as forward-mode automatic differentiation (
  - More efficient if output dimension larger than input dimension

Deep Feedforward Networks: optimization challenges

$$\text{minimize} \quad \phi(\beta) = \frac{1}{2}\sum_{i=1}^{m}(f(x_i;\beta) - y_i)^2$$

High-dimensional

- many β parameters n (due to many layers)
- **solution**: gradient-based methods
- many training samples m and (need lots of data to tune many parameters)
- **solution**: stochastic/minibatch methods (e.g., stochastic gradient descent)

Non-convex

- can get trapped in local minima
- **solution**: local minima seem to yield a “low-enough” cost-function value

Ill conditioning

- **solution**: second-order methods (but hard for NNs)

Stochastic methods

Outline

What does 'Big Data' mean for model fitting?

- In model fitting, the objective function is usually composed of a sum of m contributions:

$$\phi(\beta) = \frac{1}{m} \sum_{i=1}^{m} \phi_i(\beta)$$

  - ϕ_i: is the loss associated with the ith training example
  - ϕ: a sampling-based approximation of the expected loss
- 'Big Data' can refer to:
  - many training examples: m large
  - many parameters: n large
  - deep learning falls in this category!
- Specialized methods have been developed for these cases!
  - **stochastic/minibatch methods** (next)
  - distributed optimization (see 'Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers' by Boyd et al.)

Stochastic methods

Here, the gradient is also a sum of m contributions:

$$\nabla\phi(\beta) = \frac{1}{m}\sum_{i=1}^{m}\nabla\phi_i(\beta)$$

- **Batch methods** use this within gradient-based optimization
- **Benefit**: Preserves traditional convergence rates
- **Drawbacks**:
  - Requires accessing all m data points each iteration *(costly)*
  - Many data points are likely *redundant*
- Can we make this less expensive yet still maintain convergence?

Observations:

1. The objective is (usually) just the **sample mean** of the loss function
2. Expectations via Monte Carlo sampling converge slowly (rate $m^{-1/2}$)
3. Exact gradients aren't needed for convergence

Idea: inexpensively approximate the gradient with a *sample* of the data

Stochastic methods

Stochastic methods: compute approximate the gradient as

$$\nabla\phi(\beta) \approx \nabla\phi_i(\beta)$$

- i is a randomly chosen training example
- **Stochastic gradient descent (SGD)**: stochastic approximation to gradient descent:

$$x_{i+1} = x_k - \alpha_k \nabla\phi_i(\beta)$$

- **Benefits**:
  - each iteration is *much cheaper*
  - often observe faster rate of convergence *as a function of accessed data points*
  - a descent direction *in expectation*, i.e., $\mathbb{E}[\nabla\phi_i(\beta)] = \nabla\phi(\beta)$
- **Drawbacks**
  - slower rate of convergence *as a function of iteration* (sublinear for SGD)
  - observed slowdown as iterations progress due to noisy gradients

SGD performance in practice

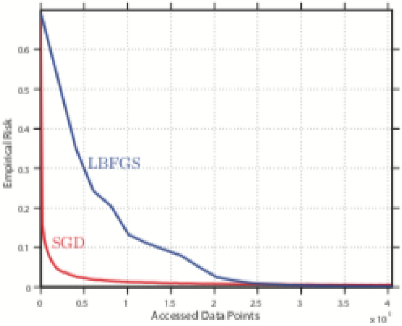


Fig. 3.1 *Empirical risk R_n as a function of the number of accessed data points (ADPs) for a batch L-BFGS method and the SG method (3.7) on a binary classification problem with a logistic loss objective and the RCV1 dataset. SG was run with a fixed stepsize of $\alpha = 4$.*

Reference: Bottou, L., Curtis, F.E. and Nocedal, J., 2018. Optimization methods for large-scale machine learning. SIAM Review, 60(2), pp.223-311.

Improving the convergence rate of stochastic methods

Noise reduction: reduce variance gradient estimate

- *Dynamic sampling*: use **minibatch** estimates of the gradient at iteration k

$$\nabla\phi(\beta) \approx \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla\phi_i(\beta),$$

  where the minibatch size $|\mathcal{S}_k|$ increases with k.
- *Gradient aggregation*: reuse recently computed gradient information
  - *Example*: stochastic variance reduced gradient (SVRD):

$$\nabla\phi(\beta) \approx \nabla\phi_i(\beta) - (\nabla\phi_i(\bar{\beta}) - \nabla\phi(\bar{\beta}))$$

  - $\bar{\beta}$: variables the last time the true batch gradient was computed

Improving the convergence rate of stochastic methods

Second-order methods: use sampled Hessian information

- **Subsampled Hessian-Free Newton Methods**: minibatch estimate of the Hessian

$$\nabla^2 \phi(\beta) \approx \frac{1}{|\mathcal{S}_k^H|} \sum_{i \in \mathcal{S}_k^H} \nabla^2 \phi_i(\beta)$$

  - Can also enforce positive definiteness via subsampled Gauss–Newton approximations
- **Subsampled Quasi-Newton Methods**:
  - typical quasi-Newton methods with stochastic estimates of the gradient