Improving and Extending Linear Models

Shyue Ping Ong

University of California, San Diego

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Overview

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Preliminaries

- In this lecture, we will look at various approaches to improving and extending simple linear models.
- It is important to note that techniques and concepts such as regularization, shrinkage and transformation of inputs are general and extend to other models.

Improving on linear models

Improving on linear models

Feature selection

- Often, we want to improve on the least squares model.
  - To improve prediction accuracy by sacrificing some bias for reduced variance.
  - To improve interpretability by reducing number of features or descriptors.
- Three main approaches:
  1. Subset selection
  2. Shrinkage methods
  3. Dimension reduction

Subset selection

Best subset selection

- Brute force approach.
- From p parameters, find the subset of k parameters that results in the smallest RSS.
- Combinatorially expensive for large p and large k.
- Note that the best subset for a larger k does not necessarily include the best subset for a smaller k.

Forward- or backward-stepwise selection

- Forward: Start with intercept, and iteratively add feature that most improves the fit.
- Backward: Start with full model, and sequentially deletes the feature with least impact on the fit.

Shrinkage methods

- Subset methods is discrete, i.e., retains/discards variables, and tends to exhibit high variance.
- Shrinkage methods are more continuous and do not suffer as much from high variability.
- Basic concept: instead of finding the parameters that minimizes the RSS only, we add a penalty term that penalizes more complex models, e.g., models with larger coefficients or larger number of coefficients. This "shrinks" the coefficients, in some cases, to 0.

Ridge regression (L_2 regularization)

$$\hat{\beta^{ridge}} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$

- $\lambda \geq 0$ is the shrinkage parameter. The larger the λ, the greater the shrinkage.
- Also equivalent to:

$$\hat{\beta^{ridge}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_j)^2$$
$$\text{subject to} \sum_{j=1}^{p} \beta_j^2 \leq t$$

Ridge regression - Key details

- Intercept (β_0) is not part of penalty term.
- Inputs should be scaled prior to performing ridge regression, typically by centering to the mean and scaling to unit variance:

$$z_j = \frac{x_j - \mu_{x_j}}{s_{x_j}}$$

LASSO (L_1 regularization)

$$\hat{\beta^{LASSO}} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

- Least Absolute Shrinkage and Selection Operator
- $\lambda \geq 0$ is the shrinkage parameter. The larger the λ, the greater the shrinkage.
- Also equivalent to:

$$\hat{\beta^{LASSO}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_j)^2$$

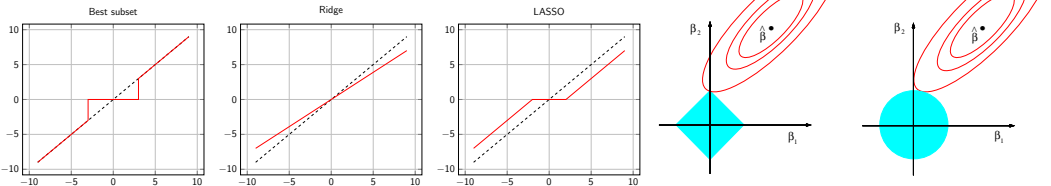
$$\text{subject to} \sum_{j=1}^{p} |\beta_j| \leq t$$

LASSO regression - Key details

- Intercept (β_0) is not part of penalty term.
- Inputs should be scaled prior to performing lasso regression, just as in ridge regression.

Subset vs ridge vs LASSO

- Consider a set of orthonormal features.
  - Ridge: proportional shrinkage. No coefficients are set to zero.
  - LASSO: "soft" thresholding. Translates coefficients by a factor, truncating at zero.
  - Best-subset: "hard" thresholding. Drops all coefficients below a certain threshold.



Other variants of shrinkage methods

- Elastic net penalty:

$$\lambda \left(\alpha \sum_{j=1}^{p} \beta_j^2 + (1-\alpha) \sum_{j=1}^{p} |\beta_j| \right)$$

- Least angle regression

Derived input directions

- General concept: transforms input $\mathbf{X}$ into a smaller subset of $\mathbf{z_m}$ and regress on $\mathbf{z_m}$
- Principal component regression:
  - Transform non-orthonormal features into orthonormal directions using Principal Component Analysis (PCA).
  - Choose M directions that have the highest eigenvalues (explains the most variance) and discards the rest.
  - Will revisit at a later lecture.

Partial Least Squares (PLS)

- Algorithm:
  1. Compute $\phi_{1j} = < \mathbf{x_j}, \mathbf{y} >$ for each j.
  2. First transformed direction $\mathbf{z_1} = \sum_j \phi_{1j} \mathbf{x_j}$, i.e., each direction is weighted by strength of effect on $\mathbf{y}$.
  3. Regress $\mathbf{y}$ on $\mathbf{z_1}$ to obtain θ_1, orthogonalize $\mathbf{x_1}, ...\mathbf{x_p}$ wrt $\mathbf{z_1}$ via $x'_j = x_j - \frac{<\mathbf{z_1}, \mathbf{x_j}>}{<\mathbf{z_1}, \mathbf{z_1}>} \mathbf{z_1}$.
  4. Repeat until $M \leq p$ coefficients are obtained.
- Finds directions with high variance and high correlation with response.

Preliminaries

- It is highly unlikely that the true function $f(X)$ is linear in X.
- In some cases, linearity is a reasonable assumption, e.g., a first order Taylor series expansion:

$$f(x) = f(a) + f'(a)(x-a) + f''(a)\frac{(x-a)^2}{2!} + f'''(a)\frac{(x-a)^3}{3!} + ...$$

- Examples where this is used in materials science - linear elasticity (Hooke's law), etc.
- More frequently, we perform a transformation of inputs to create a linear basis expansion.

General concept

- Express:

$$f(X) = \sum_{m=1}^{M} \beta_m h_m(X)$$

  where h_m is the m^{th} transformation of X.
- This is known as a linear basis expansion in X.
- The key lies in choice of the basis functions h_m.

Examples of basis expansions

- $h_m(X) = X_j^2, h_m(X) = X_i X_j$
  - Polynomial expansion to higher-order Taylor series terms.
  - No. of terms increases exponentially with degree of polynomial. For p variables, we have $O(p^2)$ square and cross-product terms in a quadratic model. For a degree d polynomial, we have $O(p^d)$.
- $h_m(X) = log(X_j), sqrt(X_j), exp(iX_j)$: non-linear transformations in X.
- $h_m(X) = I(L_m \leq X_k < U_m)$: Piece-wise division of regions of X. E.g., cubic splines.
- $h_m(X) = RBF(||X - X_m||)$: radial basis function, e.g., Gaussian.
- Typically, basis functions are used simply to allow a more flexible representation of the data. The basis functions can span a very large (sometimes infinite) set, from which a selection has to be made:
  - Restriction - Truncate the choice of basis functions using some criteria.
  - Selection - Choose basis functions that contribute significantly to the fit.
  - Regularization - Use the whole and/or very large subset and apply regularization techniques (e.g., ridge or LASSO) to restrict coefficients.

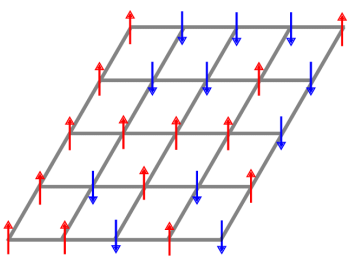
Linearization from physical laws

- Arrhenius law:

$$r = A\exp(-\frac{E_a}{RT}) \longrightarrow log(r) = log(A) - \frac{E_a}{RT}$$

- Ising model:

$$H(\sigma) = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j$$

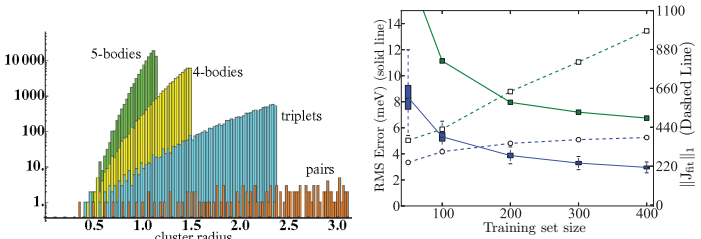


Compressive sensing for cluster expansions

- Cluster expansion of energy on lattice points:

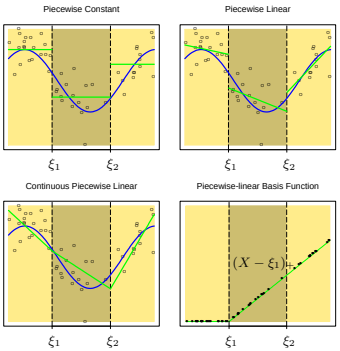
$$H(\sigma) = E_0 + \sum_f J_f \prod_f (\sigma)$$

- σ is the vector representing occupation of lattice sites, $\prod_f$ are the cluster basis functions, J_f are effective cluster interactions (ECIs).
- Compressive sensing: essentially a LASSO to solve for ECIs.[1]



Piecewise polynomials

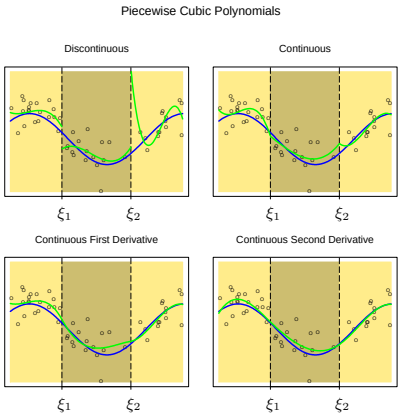
$$h_1(X) = I(X < \xi_1), h_2(X) = I(\xi_1 \leq X < \xi_2), h_3(X) = I(X \geq \xi_2)$$



Parameters:

- No. of knots
- Order of polynomial
- Continuity at knots (value, first derivative, second derivative, etc.). For a polynomial of order N, we usually want all derivatives $< N$ to be continuous.

Cubic splines



- Probably the most commonly used.
- Continuous 1st and 2nd derivatives.
- Natural cubic spline: polynomial is linear beyond boundaries.
- Smoothing spline: Use regularization to control complexity:

$$RSS(f,\lambda) = \sum_{i=1}^{N}\{y_i - f(x_i)\}^2 + \lambda \int \{f''(t)\}^2 dt$$

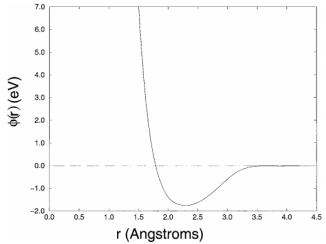
Examples of cubic spline fitting

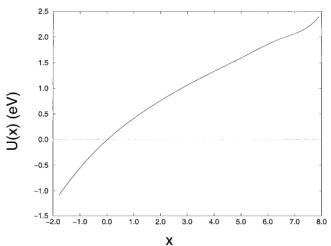
- Spline-based Modified Embedded Atom Method (MEAM)

$$E = \sum_{i<j} \phi(r_{ij}) + \sum_i U(n_i),$$

$$n_i = \sum_j \rho(r_{ij}) + \sum_{i<k,j,k!=i} f(r_{ij}) f(r_{ik}) g[cos(\theta_{jik})]$$

where ϕ, U, ρ, f and g can be approximated by cubic splines.





Demo: Cubic spline fitting in scipy

```
import numpy as np

## Import CubicSpline from scipy
from scipy.interpolate import CubicSpline

## x, y data for generating the spline fitting
x = np.arange(10)
y = np.sin(x)
## Fit the spline
cs = CubicSpline(x, y)
## Generate new x values
xs = np.arange(-0.5, 9.6, 0.1)
## Perform the interpolation on the new points
ys = cs(xs)
```

Gaussian basis functions

$$h_m(x) = \exp(-k(x - x_m)^2)$$

- Gaussian functions centered at x_m.
- Other similar types of functions include Lorentzian ($h_m(x) = \frac{1}{1+kx^2}$), Gaussian-Lorentzian, Voigtian, Pearson type IV, and beta profiles.

Example: Rietveld refinement

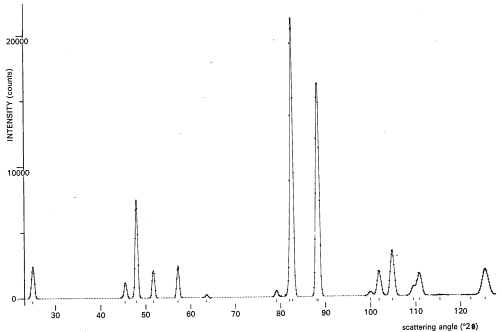


Figure: Neutron powder diffraction diagram of $CaUO_4$

- Least squares fitting of theoretical line profile to match a measured diffraction pattern (e.g., X-ray, neutron).[2]

Example: Rietveld refinement, contd.

- Peak shape function:

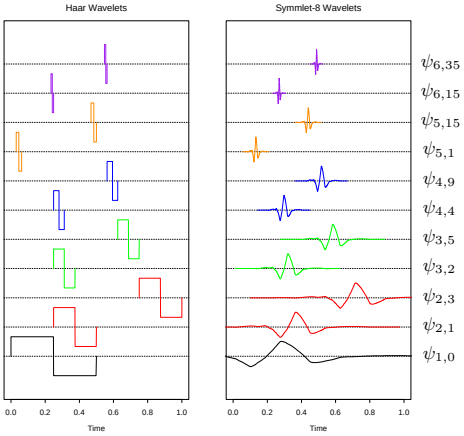
$$PSF(\theta) = \Omega(\theta) \otimes \Lambda(\theta) \otimes \Psi(\theta) + b(\theta)$$

- Ω: Instrument broadening, Λ: Wavelength dispersion, Ψ: Specimen function.
- For single phase, minimize:

$$\Phi = \sum_{i=1}^{N} w_i \left(Y_i^{obs} - \left(b_i + K \sum_{j=1}^{m} I_j y_j(x_j) \right) \right)^2$$

- where $y_j(x_j)$ is typically a pseudo-Voigt (mix of Gaussian and Lorentizan function) function.
- Note that the background (b_i) holds no useful structural information and should be minimized in experiments.

Wavelet smoothing



- Complete orthonormal basis
- Shrink and select toward **sparse** representation.
- Able to represent both time and frequency localization efficiently (Fourier basis can only do frequency localization).

Example: NMR Spectroscopy

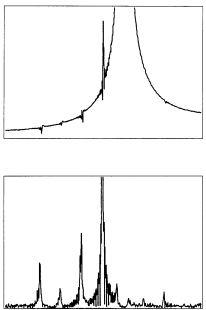
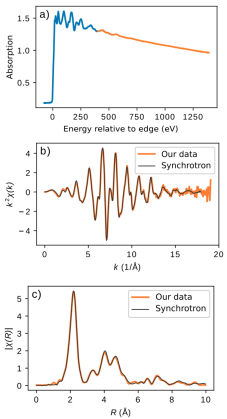


Figure: Subtraction of a large spectral line: (top) the original spectrum of polyethylene, (bottom) reconstructed spectrum after removal of CH_2 peak.[3]

Applications:

- Suppression of large unwanted spectral line (left).
- Rephasing spectrum perturbed by time-dependent magnetic field.
- Noise filtering
- Detecting phases in a mixture

Example: Fourier transform for analysis of extended X-ray absorption fine structure (EXAFS)



- (a) The extended edge (orange part) contains information of atom chemical environment.
- (b) Subtract the background, convert energy to k-space unit, and multiply the normalized intensity by k^2
- (c) Fourier transform k-space information to real space and obtain the first shell bond length.

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