# Improving and Extending Linear Models

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# Overview

# Preliminaries

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- 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

# 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)

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

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

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

$$\text{subject to} \sum_{j=1}^{p} \beta_j^2 \leq t$$

# Ridge regression - Key details

- Intercept ($\beta_0$) 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)

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

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

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

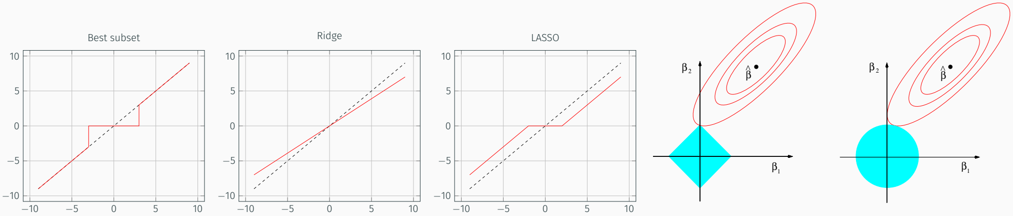
$$\text{subject to} \sum_{j=1}^{p} |\beta_j| \leq t$$

# LASSO regression - Key details

- Intercept ($\beta_0$) 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 $\theta_1$, orthogonalize $\mathbf{x_1}, \ldots \mathbf{x_p}$ 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.

# Extending linear methods

# 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:

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

- 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.

# Transformation of inputs

# 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

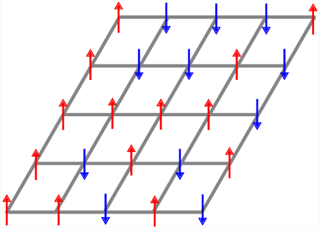
# Linearization from physical laws

- Arrhenius law:

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

- Ising model:

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

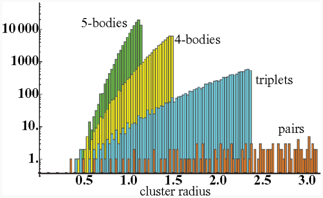


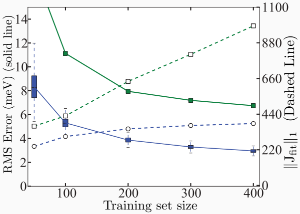
# Compressive sensing for cluster expansions

- Cluster expansion of energy on lattice points:

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

- $\sigma$ 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]

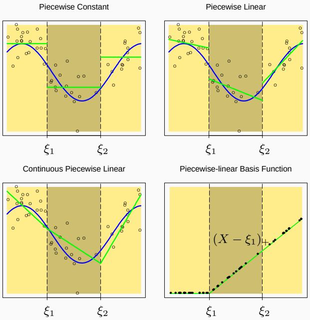


# Piece-wise polynomials

# Piecewise polynomials

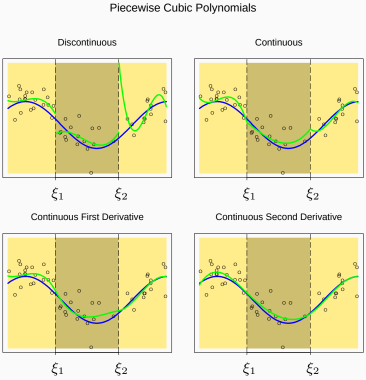
$$h_1(X) = I(X < \xi_1), h_2(X) = I(\xi_1 \leq X < \xi_2), h_3(X) = I(X \geq \xi_2)$$




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:

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

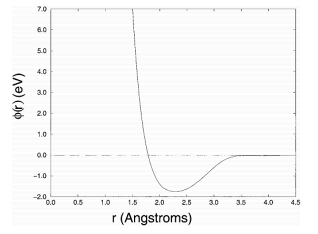
# Examples of cubic spline fitting

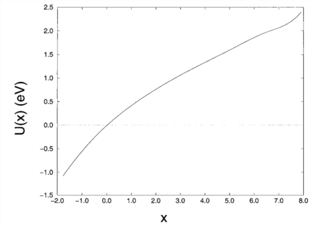
- Spline-based Modified Embedded Atom Method (MEAM)

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

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

where $\phi$, $U$, $\rho$, $f$ and $g$ can be approximated by cubic splines.



# Demo: Cubic spline fitting in scipy

```
from __future__ import annotations

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

# 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

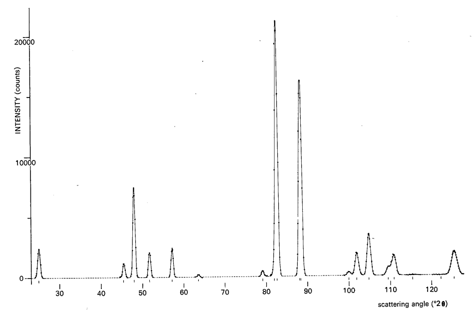



**Figure 1:** Neutron powder diffraction diagram of $CaUO_4$

- 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:

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

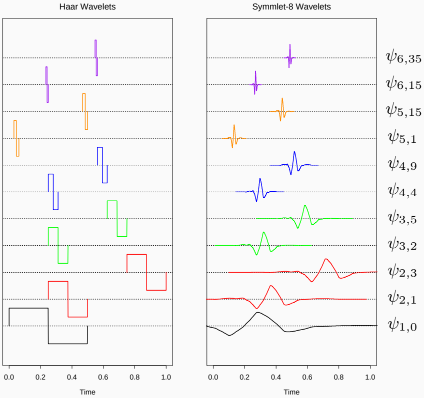
- $\Omega$: Instrument broadening, $\Lambda$: Wavelength dispersion, $\Psi$: Specimen function.
- For single phase, minimize:

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

- 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 and Fourier basis functions

# 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

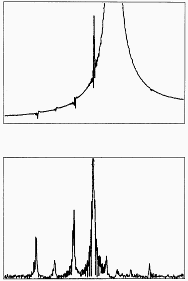
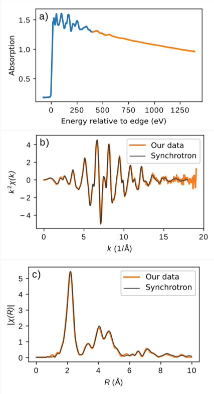


**Figure 2:** Subtraction of a large spectral line: (top) the original spectrum of polyethylene, (bottom) reconstructed spectrum after removal of $CH_2$ peak.[3]

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.

# Bibliography i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# The End