Linear Methods

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6. Transformation of inputs
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Preliminaries

- We will go very deep into linear models.
- Most of you probably have seen linear models in some form, but we will start from scratch to further illustrate key concepts such as bias and variance.
- We will then discuss techniques such as regularization and transformation of inputs in the context of linear methods.

Notation

- Capital letters, e.g., X denote variables.
- Lower-case letters e.g., x, denote observations.
- Dummy index j to denotes different variables, e.g., X_j
- Dummy index i to denotes different observations, e.g., x_i
- Bolded variables are vector/matrices, e.g., $\mathbf{y}$, $\mathbf{X}$

Linear Regression

Linear Regression

Simplest possible model between target and feature

$$Y = f(X_1, X_2, ..., X_p) = \beta_0 + \sum_{j=1}^{p} \beta_j X_j$$

X_j can be:

- Quantitative inputs
- Transformations of quantitative inputs, e.g., log, exp, powers, etc. Basis expansions, e.g., $X_2 = X_1^2$, $X_3 = X_1^3$
- Interactions between variables
- Encoding of levels of inputs

Supervised learning

- Given a set of paired observations $\{x_{ij}, y_i\}$, what are the model parameters (in this case, the coefficients β_j) that are "optimal"?
- "Optimal" is typically defined as minimization of some **loss function** (also known as **cost function**) that measures the error of the model.

Least squares regression

Consider the simple case of

$$Y = \beta_0 + \beta_1 X_1$$

In least squares regression, the loss function is defined as the sum squared error given the N observations:

$$\begin{aligned} L(Y, \hat{f}(X)) &= \sum_{i=1}^{N} (y_i - f(x_i))^2 \\ &= \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_{i1})^2 \end{aligned}$$

What are the optimal parameters β_0 and β_1?

$$
\begin{aligned}
\frac{\partial L}{\partial \beta_0} &= \sum_{i=1}^{N} 2(y_i - \beta_0 - \beta_1 x_{i1})(-1) = 0 \\
\implies & \sum_{i=1}^{N} y_i = N\beta_0 + \sum_{i=1}^{N} \beta_1 x_{i1} \\
\implies & \beta_0 = \bar{y} - \beta_1 \bar{x_1} \\
\frac{\partial L}{\partial \beta_1} &= \sum_{i=1}^{N} 2(y_i - \beta_0 - \beta_1 x_{i1})(-x_{i1}) = 0 \\
\implies & \beta_1 = \frac{\sum_{i=1}^{N} x_{i1} y_i - N\bar{x_1}\bar{y}}{\sum_{i=1}^{N} x_{i1}^2 - N\bar{x_1}^2}
\end{aligned}
$$

Reformulating the general multiple linear regression as a vector equation...

Considering N observations of

$$y_i = \beta_0 + \beta_1 x_{i1} + +\beta_2 x_{i2} + \ldots + \beta_p x_{ip}$$

Let

$$\mathrm{y} = \begin{pmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \ldots \\ \beta_p \end{pmatrix}, \mathrm{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \ldots & x_{1p} \\ 1 & x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & & & & \\ 1 & x_{N1} & x_{N2} & \ldots & x_{Np} \end{pmatrix},$$

So,

$$\mathrm{y} = \mathrm{X}\boldsymbol{\beta}$$

Note that y is a $N \times 1$ vector, $\boldsymbol{\beta}$ is a $(p+1) \times 1$ vector, and X is a $N \times (p+1)$ matrix.

Reformulating the general multiple linear regression as a vector equation...

$$L = RSS = (\mathrm{y} - \mathrm{X}\boldsymbol{\beta})^T(\mathrm{y} - \mathrm{X}\boldsymbol{\beta})$$

Assuming (for the moment) that X has full column rank, and hence $\mathrm{X}^T\mathrm{X}$ is positive definite, It can be shown using the same principles that the following unique solution for $\boldsymbol{\beta}$ is:

$$\begin{aligned} \hat{\boldsymbol{\beta}} &= (\mathrm{X}^T\mathrm{X})^{-1}\mathrm{X}^T\mathrm{y} \\ \hat{\mathrm{y}} &= \mathrm{X}\hat{\boldsymbol{\beta}} = \mathrm{X}(\mathrm{X}^T\mathrm{X})^{-1}\mathrm{X}^T\mathrm{y} \end{aligned}$$

Graphic representation of MLR with two dependent variables

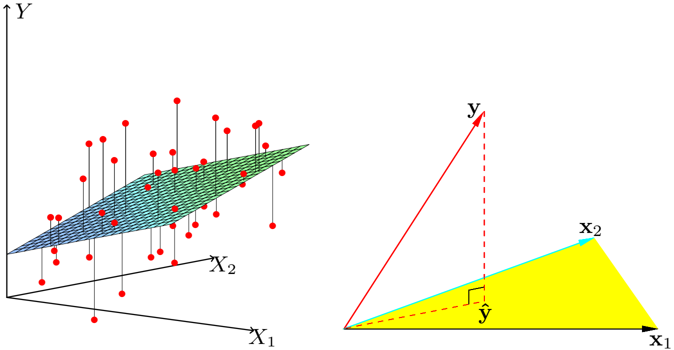


Figure: MLR minimizes sum square of residuals. The projection $\hat{y}$ represents the vector of the least squares predictions onto the hyperplane spanned by the input vectors x_1 and x_2. [2].

Validity of least squares criterion

- Observations are independently drawn at random.
- Variance of y is constant given by σ^2.

$$\mathrm{var}(\hat{\beta}) = (\mathsf{X}^T\mathsf{X})^{-1}\sigma^2$$

- and σ is estimated using:

$$\sigma^2 = \frac{1}{N-p-1}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Hypothesis Testing for Coefficients

- To derive insights into a model, we often want to know which of the input parameters are the most relevant to the target.
- Under assumptions of the errors in y follow a Gaussian distribution $N(0, \sigma^2)$, the errors in $\hat{\boldsymbol{\beta}}$ also have a Gaussian distribution $N(\beta, (\mathrm{X}^T\mathrm{X})^{-1}\sigma^2)$
- Hypothesis testing can be carried out for whether a particular β_j is 0 using the following test statistic:

$$t_j = \frac{\hat{\boldsymbol{\beta}}_{\boldsymbol{j}}}{\sigma\sqrt{v_j}}$$

where v_j is the jth diagonal element of $(\mathrm{X}^T\mathrm{X})^{-1}$. t_j has a t distribution with $N - p - 1$ degrees of freedom (dof).

Hypothesis Testing for Groups of Coefficients

- More often, we want to test groups of coefficient for significance. E.g., to the k levels of a categorical variable.
- We will use the following F statistic:

$$F = \frac{(\mathrm{RSS}_0 - \mathrm{RSS}_1)/(p_1 - p_0)}{\mathrm{RSS}_1/(N - p_1 - 1)}$$

where RSS_0 is the RSS of the larger model with $p_0 + 1$ parameters and RSS_1 is the RSS of the smaller model with $p_1 + 1$ parameters with $p_0 - p_1$ parameters set to zero. The F statistic has a distribution of $F_{p_1 - p_0, N - p_1 - 1}$.

Gauss-Markov Theorem

- Consider the estimator $\hat{\theta}$ for a variable θ.

$$\begin{aligned} \mathrm{MSE} &= E(\hat{\theta} - \theta)^2 \\ &= \mathrm{var}(\hat{\theta}) + [E(\hat{\theta}) - \theta]^2 \end{aligned}$$

- The MSE can be broken down into the variance of the estimate itself and the square of the bias.

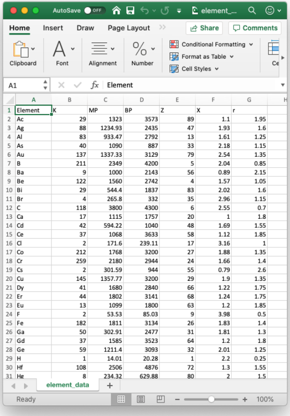
Gauss-Markov Theorem

The least squares estimator has the smallest variance among all linear *unbiased* estimators.

- However, there can be estimators that are biased with smaller MSE.

Example materials data

- Target: Bulk modulus of elements (from Materials Project)
- Candidate features:
    - Melting point (MP)
    - Boiling point (MP)
    - Atomic number (Z)
    - Electronegativity (χ)
    - Atomic radius (r)
- Question: Why these features?
- We will add some transformations of these inputs as well, i.e., the square and square root of the electronegativity and atomic radius.



Element	K	MP	BP	Z	X	r
Ac	29	1323	3573	89	1.1	1.95
Ag	88	1234.93	2435	47	1.93	1.6
Al	83	933.47	2792	13	1.61	1.25
As	40	1090	887	33	2.18	1.15
Au	137	1337.33	3129	79	2.54	1.35
B	211	2349	4200	5	2.04	0.85
Ba	9	1000	2143	56	0.89	2.15
Be	122	1560	2742	4	1.57	1.05
Bi	29	544.4	1837	83	2.02	1.6
Br	4	265.8	332	35	2.96	1.15
C	118	3800	4300	6	2.55	0.7
Ca	17	1115	1757	20	1	1.8
Cd	42	594.22	1040	48	1.69	1.55
Ce	37	1068	3633	58	1.12	1.85
Cl	2	171.6	239.11	17	3.16	1
Co	212	1768	3200	27	1.88	1.35
Cr	259	2180	2944	24	1.66	1.4
Cs	2	301.59	944	55	0.79	2.6
Cu	145	1357.77	3200	29	1.9	1.35
Dy	41	1680	2840	66	1.22	1.75
Er	44	1802	3141	68	1.24	1.75
Eu	13	1099	1800	63	1.2	1.85
F	2	53.53	85.03	9	3.98	0.5
Fe	182	1811	3134	26	1.83	1.4
Ga	50	302.91	2477	31	1.81	1.3
Gd	37	1585	3523	64	1.2	1.8
Ge	59	1211.4	3093	32	2.01	1.25
H	1	14.01	20.28	1	2.2	0.25
Hf	108	2506	4876	72	1.3	1.55
Hg	8	234.32	629.88	80	2	1.5

Using pandas for easy data manipulation

```python
import pandas as pd
# Read in data and set first column as index.
data = pd.read_csv("element_data.csv", index_col=0)
# Generate transformations as additional columns.
data["X^2"] = data["X"] ** 2
data["sqrt(X)"] = data["X"] ** 0.5
data["r^2"] = data["r"] ** 2
data["sqrt(r)"] = data["r"] ** 0.5
# Define our features, which is all the columns
# excluding K, which is the target.
features = [c for c in data.columns if c != "K"]
x = data[features]
y = data["K"]
```

Recommendation: Go through the 10 minute guide to pandas.

MLR in scikit-learn

```
from sklearn import linear_model
reg = linear_model.LinearRegression()
reg.fit(x, y)
print(ref.coef_)
print(reg.intercept_)
```

- Note that x should contain the features only - there is no need to add a 1 column for the intercept. By default, the parameter fit_intercept in sklearn.linear_model.LinearRegression is True. You can set it to False to do a MLR without intercept.
- Documentation: link.

Model selection

Model selection

Model performance

- We will take a brief digression into model assessment and selection before continuing on to other linear methods.
- Model performance is related to its performance on *independent test data*, i.e., one cannot simply report a model's performance on training data alone.
- Note that this section is deliberately limited to high level concepts that are needed to continue further in exploration of linear methods. A more detailed discussion will be performed in later lectures.

Typical measures of model performance

- Mean squared error (MSE):

$$L(Y, \hat{f}(X)) = \frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i))^2$$

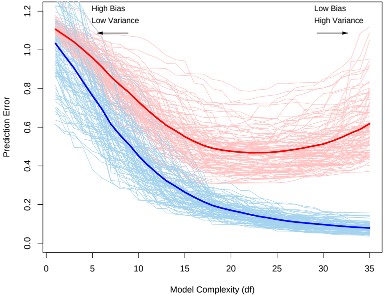
- Mean absolute error (MAE):

$$L(Y, \hat{f}(X)) = \frac{1}{N}\sum_{i=1}^{N}|y_i - f(x_i)|$$

- Test error: L over independent test set.
- Training error: L over training set.

Training and test errors with model complexity

- Model complexity increases as the number of parameters increases (e.g., number of independent variables in MLR).
- Training errors **always** decrease with increasing model complexity.
- However, test errors do not have a monotonic relationship with model complexity. Test errors are high when model complexity is too low (underfitting) or too high (overfitting).



Training, validation and test data

- Model selection: estimating the performance of different models in order to choose the best one.
- Model assessment: having chosen a final model, estimating its prediction error (generalization error) on new data.
- Ideal data-rich situation: Divide data into three parts:
  - Training set: For training the model.
  - Validation set: For estimating prediction error to select the model.
  - Test set: For assessing the generalization error of the final model.
- Typical training:validation:test split is 50:25:25 or 80:10:10, or in very data-poor situations, maybe even 90:5:5.
- Note that at no point in the model fitting process should the test set be "seen".

K-fold cross validation (CV)

- Simplest and most widely used approach for model validation.
- Data set is split into K buckets (usually by random).
- Typical values of K is 5 or 10. $K = N$ is known as “leave-one-out” CV.

Train	Train	Validate	Train	Train

- CV score is computed on the validate data set after training on the train data:

$$CV(\hat{f}^{-k(i)}, \alpha) = \frac{1}{N_{k(i)}} \sum_{i=1}^{N_{k(i)}} L(y_i, \hat{f}^{-k(i)}(x_i, \alpha))$$

- assuming the k^{th} data bucket has $N_{k(i)}$ data points and $\hat{f}^{-k(i)}$ refers to the model fitted with the k^{th} data left out ($N - N_{k(i)}$ data in fitting).

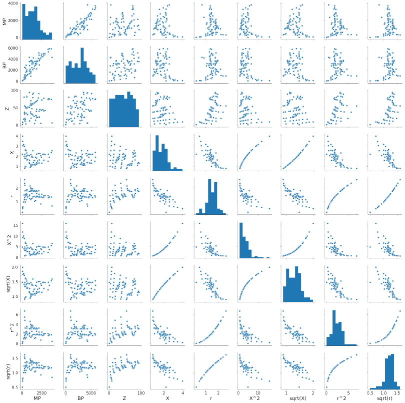
CV in scikit-learn

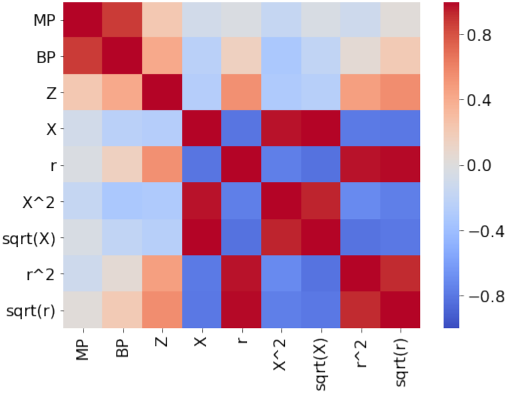
```
from sklearn.model_selection import cross_validate, KFold
kfold = KFold(n_splits=5, shuffle=True, random_state=42)
cv_results = cross_validate(ridge, z, y, cv=kfold)
```

- Note that we have customized the KFold object passed to the cross_validate method. The reason is that our element data is non-random by default. So we want to perform shuffling prior to doing the splits.
- Documentation: link.

Characteristics of the example materials dataset

- Before proceeding further, let us try to tease out some aspects of the dataset.
- Quite clearly, there are correlations between some sets of variables.
- In other words, the input features are **non-orthonormal** with each other.





Beyond least squares

Beyond least squares

Model 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)

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

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

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

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

Ridge regression - Key details

- Intercept (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)

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

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

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

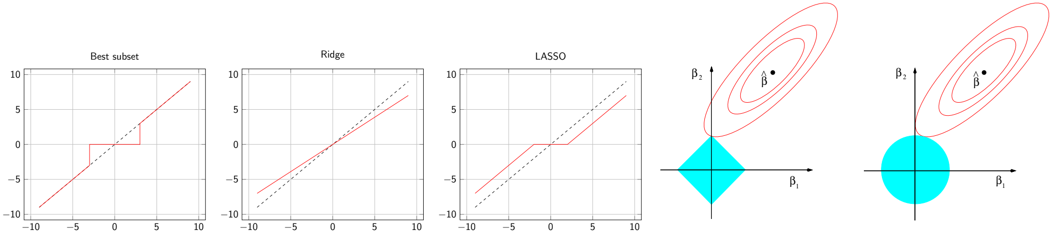
$$\text{subject to} \sum_{j=1}^{p} |\beta_j| \leq t$$

LASSO regression - Key details

- Intercept (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 X into a smaller subset of $\mathrm{z_m}$ and regress on $\mathrm{z_m}$
- 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 $\phi_{1i} =< \mathrm{x_j}, \mathrm{y} >$ for each j.
  2. First transformed direction $\mathrm{z}_1 = \sum_j \phi_{1i}\mathrm{x_j}$, i.e., each direction is weighted by strength of effect on y.
  3. Regress y on z_1 to obtain θ_1, orthogonalize $\mathrm{x}_1, \ldots \mathrm{x_p}$ wrt z_1 via $x_j' = x_j - \frac{<\mathrm{z}_1, \mathrm{x_j}>}{<\mathrm{z}_1, \mathrm{z}_1>}\mathrm{z}_1$.
  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:

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

- 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.

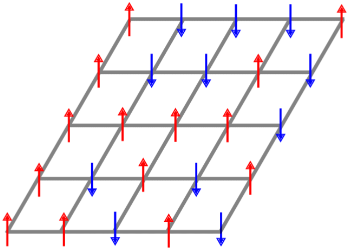
Linearization from physical laws

- Arrhenius law:

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

- Ising model:

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

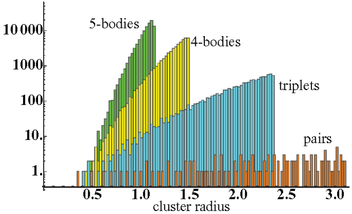


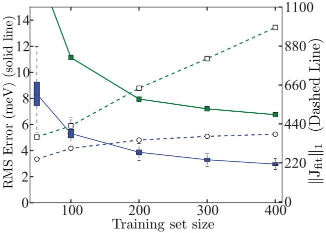
Compressive sensing for cluster expansions

- Cluster expansion of energy on lattice points:

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

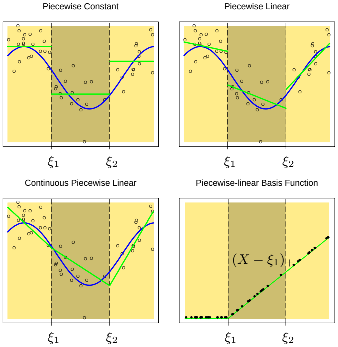
- σ is the vector representing occupation of lattice sites, $\prod_f$ are the cluster basis functions, J_f are effective cluster interactions (ECIs).
- Compressive sensing: essentially a LASSO to solve for ECIs.[3]





Piecewise polynomials

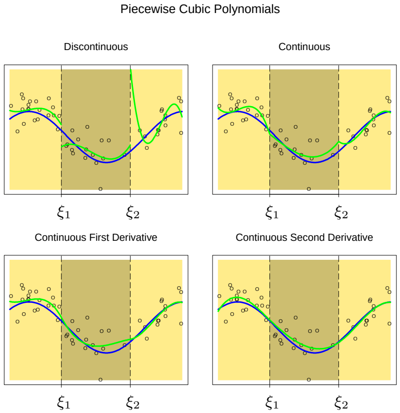
$$h_1(X) = I(X < \xi_1), h_2(X) = I(\xi_1 \leq X < \xi_2), h_3(X) = I(X \geq \xi_2)$$



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:

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

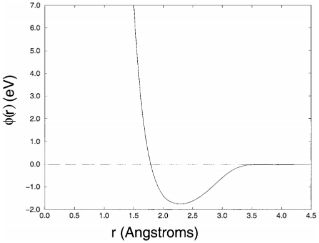
Examples of cubic spline fitting

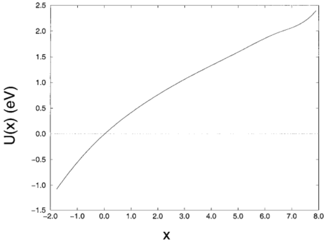
- Spline-based Modified Embedded Atom Method (MEAM)

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

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

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

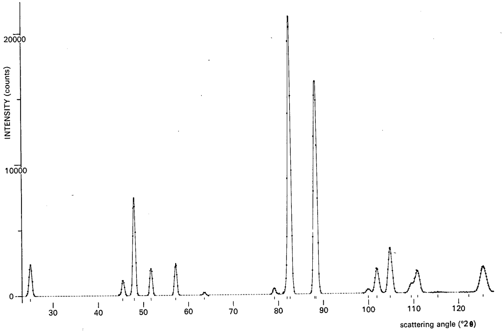


Figure: Neutron powder diffraction diagram of $CaUO_4$

- Least squares fitting of theoretical line profile to match a measured diffraction pattern (e.g., X-ray, neutron).[4]

Example: Rietveld refinement, contd.

- Peak shape function:

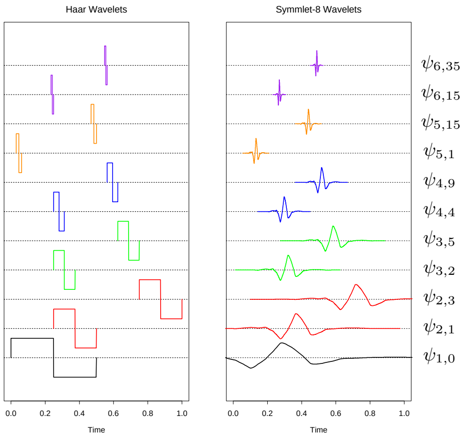
$$PSF(\theta) = \Omega(\theta) \otimes \Lambda(\theta) \otimes \Psi(\theta) + b(\theta)$$

- 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

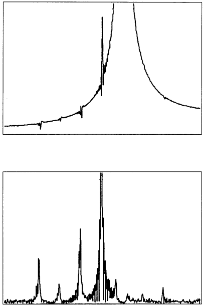
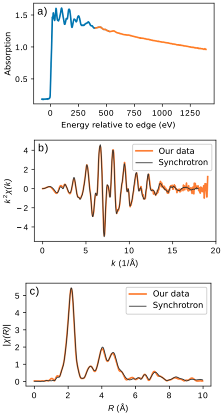


Figure: Subtraction of a large spectral line: (top) the original spectrum of polyethylene, (bottom) reconstructed spectrum after removal of CH_2 peak.[1]

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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