Tikhonov regularization: general formulation

$$J_\lambda(x) = \|Ax-b\|_2^2 + \lambda^2 \|L(x-x_0)\|_2^2$$

where x_0 denotes a prior estimate to the true solution (initial guess) and

$L \in \mathbb{R}^{p\times n}$, $p \leq n$. Typically, L is the identity matrix or a banded matrix that represents an approximation of the first or second order derivative.

An approximation to the first derivative is given by the matrix

$$L_1 = \frac{1}{\Delta x}\begin{pmatrix} -1 & 1 & & \\ & -1 & 1 & \\ & & \ddots & \ddots \\ & & -1 & 1 \end{pmatrix} \in \mathbb{R}^{(n-1)\times n}$$

$$L_1 x = \frac{1}{\Delta x}\begin{bmatrix} x_2 - x_1 \\ \vdots \\ x_{i+1} - x_i \\ x_n - x_{n-1} \end{bmatrix}$$

An approximation to the second order derivative is given by

$$L_2 = \frac{1}{(\Delta x)^2}\begin{pmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \end{pmatrix} \in \mathbb{R}^{(n-2)\times n}$$

$$L_2 x = \frac{1}{(\Delta x)^2}\begin{bmatrix} x_1 - 2x_2 + x_3 \\ \vdots \\ x_i - 2x_{i+1} + x_{i+2} \\ \vdots \\ x_{n-2} - 2x_{n-1} + x_n \end{bmatrix} \in \mathbb{R}^{n-2}$$

in general, a combination of the derivative operators may be considered

e.g., $$J_\lambda(x) = \|Ax - b\|_2^2 + \Omega(X)$$

where $\Omega(x)$ is a "Sobolev norm"

$$\Omega(X) = \lambda_0^2 \|x - x_0\|^2 + \lambda_1^2 \|L_1(x - x_0)\|^2 + \lambda_2^2 \|L_2(x - x_0)\|^2$$

<u>Remark</u> if $L \in \mathbb{R}^{n \times n}$ is a nonsingular matrix then minimization of

$$J_\lambda(x) = \|Ax - b\|_2^2 + \lambda^2 \|L(x - x_0)\|_2^2$$

may be reduced to the standard form using a change of variable

$$\tilde{x} = L(x - x_0)$$

then $x = L^{-1}\tilde{x} + x_0$

and an equivalent problem for $\tilde{x}$ is

$$\tilde{J}_\lambda(\tilde{x}) = \|\tilde{A}\tilde{x} - \tilde{b}\|_2^2 + \lambda^2 \|\tilde{x}\|_2^2$$

where $\tilde{A} \stackrel{def}{=} AL^{-1}$

$\tilde{b} \stackrel{def}{=} -Ax_0 + b = b - Ax_0$

Notice that $J_\lambda(x)$ may be expressed as

$$J_\lambda(x) = \left\| \begin{pmatrix} A \\ \lambda L \end{pmatrix} x - \begin{pmatrix} b \\ \lambda L x_0 \end{pmatrix} \right\|_2^2$$

with $\begin{pmatrix} A \\ \lambda L \end{pmatrix} \in \mathbb{R}^{(m+p)\times n}$, $\begin{pmatrix} b \\ \lambda L x_0 \end{pmatrix} \in \mathbb{R}^{m+p}$

thus
$$x_\lambda = \arg\min_x J_\lambda(x)$$

if and only if x_λ solves the linear system given by the normal equations

$$(A^T A + \lambda^2 L^T L)x = A^T b + \lambda^2 L^T L x_0$$

in addition, the solution is unique if and only if the null spaces of A and L intersect trivially,

$$\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$$