Fused Multi-Modal Electron Microscopy Pseudo Code

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Algorithm 1 Multi-Modal 2D Data Fusion (DOI: /10.1038/s41524-021-00692-5)

Objective Function: $\Psi(\boldsymbol{x}) = \frac{1}{2}\left\| \sum_i \boldsymbol{x}_i^{\gamma} - \boldsymbol{b}_H \right\|_2^2 + \lambda_{PS} \sum_i \left(\mathbf{1}^T \boldsymbol{x}_i - \boldsymbol{b}_i^T \log(\boldsymbol{x}_i + \varepsilon)\right) + \lambda_{TV} \sum_i \|\boldsymbol{x}_i\|_{\mathrm{TV}}$

Input: $b_h \in \mathbb{R}^{n_x \cdot n_y} \rightarrow$ HAADF Micrograph (Image Dimensions: $n_x \times n_y$)
Input: $b_c \in \mathbb{R}^{n_e \cdot n_x \cdot n_y} \rightarrow$ Raw Chemical Maps (Total # of Elements: n_e)
Output: $\boldsymbol{x} \in \mathbb{R}^{n_e \cdot n_x \cdot n_y} \rightarrow$ Concatenated Vector of Recovered Maps

$N_{\mathrm{iter}} = 200, ng = 15$
$\lambda_{MM} = \frac{1}{n_e}, \lambda_{PS} = 5 \cdot 10^{-3}, \lambda_{TV} = 0.1$
$\boldsymbol{x}_i^0 = b_c$ (Initialize first iterate as raw chemical maps)
for $k = 1, Niter$ **do** (Main Loop)
    $\boldsymbol{x}^k = \boldsymbol{x}^k - (\lambda_{MM} \nabla_{\boldsymbol{x}} \Psi_1(\boldsymbol{x}^k) + \lambda_{PS} \nabla_{\boldsymbol{x}} \Psi_2(\boldsymbol{x}^k))$
    for $i, \ldots, n_e$ **do**
        $\boldsymbol{x}_e^k = \mathrm{TV\_GP\_2D}(\boldsymbol{x}_e^k, \lambda_{TV}, ng)$
    end for
end for
return $\boldsymbol{x}^{Niter}$

$\nabla_{\boldsymbol{x}} \Psi_1(\boldsymbol{x}) = -\gamma \mathrm{diag}\big(\boldsymbol{x}^{\gamma-1}\big) \boldsymbol{A}^T \big(\boldsymbol{b}_H - \boldsymbol{A}\boldsymbol{x}^{\gamma}\big)$
$\nabla_{\boldsymbol{x}} \Psi_2(\boldsymbol{x}) = \mathbf{1} - \boldsymbol{b} \oslash (\boldsymbol{x} + \varepsilon)$
$\oslash$ is element wise division

Algorithm 2 2D Gradient Projection (GP) Method (DOI: 10.1109/TIP.2009.2028250)

Input: $\boldsymbol{b} \in \mathbb{R}^{n_x \times n_y} \rightarrow$ 2D Image, $\lambda \rightarrow$ Regularization Parameter, $ng \rightarrow$ Number of Iterations
Output: $\boldsymbol{x}^* \rightarrow$ Optimal Solution

function TV_GP_2D($\mathbf{x}, \lambda, ng$)
  $\boldsymbol{p}_x^0 = \mathbf{0} \in \mathbb{R}^{(m-1)\times n} \quad \boldsymbol{p}_y^0 = \mathbf{0} \in \mathbb{R}^{m\times n-1}$
  for $k = 1, ng$ **do** (Main Loop)
    $(\boldsymbol{p}_x^k, \boldsymbol{p}_y^k) = P_{\mathcal{P}}\Big[(\boldsymbol{p}_x^{k-1}, \boldsymbol{p}_y^{k-1}) + \frac{1}{8\lambda}\mathcal{L}^T(P_C[\boldsymbol{b} - \lambda\mathcal{L}(\boldsymbol{p}_x^{k-1}, \boldsymbol{p}_y^{k-1})]\Big]$
  end for
  return $\boldsymbol{x}^* = P_C[\boldsymbol{b} - \lambda\mathcal{L}(\boldsymbol{p}_x^{ng}, \boldsymbol{p}_y^{ng})]$
end function

function $\mathcal{L}(\boldsymbol{p}$,$\boldsymbol{q})$
  for $i = 1, \ldots, n_x$ **do**
    for $j = 1, \ldots, n_y$ **do**
      if $i == 0$ or $i == n_x$ **do** $p_{i,j} = 0$
      if $j == 0$ or $j == n_t$ **do** $q_{i,j} = 0$
      $\mathcal{L}(\boldsymbol{p}, \boldsymbol{q})_{i,j} = p_{i,j} + q_{i,j} - p_{i-1,j} - q_{i,j-1}$
    end for
  end for
  return $\mathcal{L}(\boldsymbol{p}, \boldsymbol{q})_{i,j}$
end function

function $\mathcal{L}^T(\boldsymbol{x})$
  for $i = 1, \ldots, n_x - 1$ **do**
    for $j = 1, \ldots, n_y - 1$ **do**
      $p_{i,j} = x_{i,j} - x_{i+1,j}$
      $q_{i,j} = x_{i,j} - x_{i,j+1}$
    end for
  end for
  return $(\boldsymbol{p}, \boldsymbol{q})$
end function

function $P_C(\boldsymbol{x})$
  return $\max\{0, \boldsymbol{x}\}$
end function

function $P_{\mathcal{P}}(\boldsymbol{p}, \boldsymbol{q})$
  for $i = 1, \ldots, n_x - 1$ **do**
    for $j = 1, \ldots, n_y - 1$ **do**
      $p_{i,j} = \frac{p_{i,j}}{\max\{1, \sqrt{p_{i,j}^2 + q_{i,j}^2}\}}$
      $q_{i,j} = \frac{q_{i,j}}{\max\{1, \sqrt{p_{i,j}^2 + q_{i,j}^2}\}}$
    end for
  end for
  return $(\boldsymbol{p}, \boldsymbol{q})$
end function